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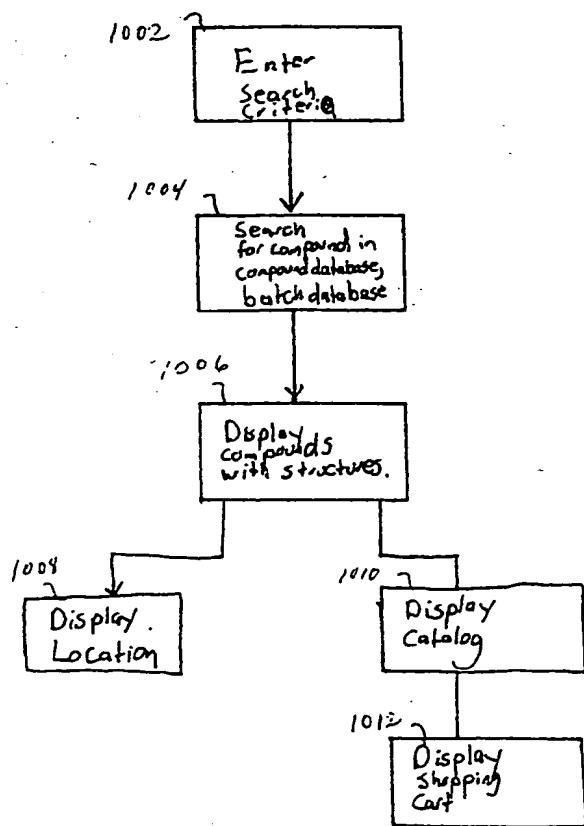
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(54) Title: CHEMICAL COMPOUND INFORMATION SYSTEM

(57) Abstract

Systems and methods for managing chemical compound information. Chemical compound tracking and purchasing systems may be provided. A user interface (1002) allows for queries to identify compounds (1004) available internally to the organization and for orders from external sources for compounds that are unavailable internally. Background processing of compound characteristics as stored in a chemical compound database (1004) may be provided (1006).



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CHEMICAL COMPOUND INFORMATION SYSTEM

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BACKGROUND OF THE INVENTION

The present invention relates to information systems and more particularly to information systems for chemical compounds.

Operation of the modern chemical laboratory environment requires the management of large numbers of chemical compound containers. These containers may be dispersed over thousands of locations. A researcher or chemist desiring a given chemical compound may be aware of chemical compounds found at his or her location or possibly at nearby locations but is likely to be unaware of chemical compounds available within his or her organization. He or she may conduct a search by physically scanning available contents at many locations or by making successive telephone calls to personnel throughout the organization. It may be more time efficient and thus cheaper to simply order the chemical compound from an external source even if the chemical compound is already available internally.

Even ordering from an external source is complicated by the need to search through numerous supplier catalogs which may not be up to date. After locating the catalog information, completing an order generally requires contacting the supplier by telephone during the supplier's business hours.

A related management problem concerns collecting and maintaining information on the characteristics of chemical compounds. For the purpose of identifying chemical compounds for particular purposes including pharmaceutical purposes, it would be desirable to maintain a chemical compound database that stores for each of many chemical compounds information including: 1) the three dimensional structure of the compound, 2) identification of pharmacophores of the compound, and 3) a specification of the compound structure that does not include disconnected salt fragments.

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SUMMARY OF THE INVENTION

By virtue of the present invention, systems and methods for managing chemical compound information are provided. One embodiment provides a chemical compound tracking and purchasing system. A container database is maintained identifying chemical compound containers available within an organization. A integrated user interface

allows for queries to identify compounds available internally to the organization and for orders from external sources for compounds that are unavailable internally.

Another embodiment of the invention provides background processing of compound characteristics as stored in a chemical compound database. When a chemical compound is registered to a database, its two-dimensional chemical structure is also registered. One or more autonomous processes take this two-dimensional chemical structure as an input to generate additional compound characteristic information to add to the compound database. For example, a first autonomous process may remove salts from stored two-dimensional structures. The removal of salts facilitates searching for useful compounds because salt substructures do not normally affect the ability of one compound to bond with another. A second autonomous process may remove protective groups from the stored structures. These are groups that cleave during synthesis and it is useful to remove them from the compound database to facilitate the evaluation of database products. A third autonomous process may determine a possible three-dimensional structure for each compound, an example of information useful in identifying compounds having desired pharmaceutical characteristics. A fourth autonomous process may identify pharmacaphoric groupings in the stored two-dimensional structures. Knowledge of the pharmacaphores found within each compound greatly facilitates searching for compounds having desired pharmaceutical characteristics.

Another embodiment of the present invention provides for chemical compound registration system having a web-based interface. The web-based interface facilitates entering information about chemical compounds from any location on a network.

A further understanding of the nature and advantages of the inventions herein may be realized by reference to the remaining portions of the specification and the attached drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 depicts a computer system suitable for implementing one embodiment of the present invention.

Fig. 2 depicts a computer network suitable for implementing one embodiment of the present invention.

Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to one embodiment of the present invention.

Fig. 4 is a flowchart describing steps of an overall background process for enriching a chemical compound database in the background according to one embodiment of the present invention.

Fig. 5 is a flowchart describing steps of removing salts from a chemical compound according to one embodiment of the present invention.

Fig. 6 depicts a compound with pharmacaphoric groupings marked and with a salt removed.

Fig. 7 depicts a simplified representation of a laboratory facility.

Fig. 8 depicts a scanner as would be used in one embodiment of the present invention.

Fig. 9 depicts a flowchart describing steps of tracking chemical compound containers according to one embodiment of the present invention.

Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention.

Figs. 11A-11F depict a user interface for locating and purchasing chemical compounds according to one embodiment of the present invention.

Fig. 12 depicts a configuration of pharmacaphoric groupings.

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DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides a chemical compound information system. In certain embodiments, the information system includes a chemical compound tracking and purchase system. In certain other embodiments, the chemical compound information system includes a chemical compound registry for registering information about new compounds. This registry may have a web-based interface. Once compounds are registered to a database, background processing may enrich the database with useful information about the compounds such as, e.g., three-dimensional structure, pharmacaphoric groupings, and information about included salts.

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Representative Hardware

Fig. 1 shows basic subsystems of a computer system suitable for use with the present invention. In Fig. 1, computer system 10 includes bus 12 which interconnects major subsystems such as central processor 14, system memory 16, input/output (I/O) controller 18, an external device such as a printer 20 via parallel port 22, display screen 24 via display adapter 26, serial port 28, keyboard 30, fixed disk drive 32 and floppy disk drive 33. Many other devices can be connected such as scanning device 34 connected via I/O controller 18, a network interface 35, a mouse 38 connected via serial port 28. Many other devices or subsystems (not shown) may be connected in a similar manner. Also, it is not necessary for all of the devices shown in Fig. 1 to be present to practice the present invention, as discussed below. The devices and subsystems may be interconnected in different ways from that shown in Fig. 1. The operation of a computer system such as that shown in Fig. 1 is readily known in the art and is not discussed in detail in the present application. Source code to implement the present invention may be operably disposed in system memory 16 or stored on storage media such as fixed disk 32 or floppy disk 33A.

Fig. 2 depicts a computer network 200 suitable for implementing the present invention. A central station 202 maintains databases as described herein. Central station 202 is preferably a Unix or Windows NT server such as an ORIGIN 2000 server available from Silicon Graphics, Inc. of Mountain View, California. Central station 202 operates databases as described below and preferably provides external access to these databases using standard well-known Internet protocols such as HTTP. Database operation may also be divided among multiple central stations.

A plurality of remote stations 204 may access the databases of central station 202 using HTTP. Database access may be for searching for needed compounds or for registering new compounds. Remote stations 204 operate standard web browsing software such as Netscape Navigator or Microsoft Internet Explorer. Remote stations 204 may be implemented on a wide variety of computer platforms that support such browsing software. Any time of network may interconnect central station 202 including LANs, WANs, the Internet, an intranet, or any combination of these.

Databases Operated

A chemical compound information system according to the present invention may maintain various databases. A chemical compound database may include records corresponding to individual chemical compounds. Each record includes one or more of the representative fields shown in Table 1.

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TABLE 1

FIELD	INFORMATION
MOLREGNO	Unique registration number for molecule
MOLNAME	Molecule name
CONV_NAME	Conventional name
IUPAC_NAME	IUPAC name
MOLFORMULA	Molecular formula
MIN_MWT	Minimum molecular weight
MAX_MWT	Maximum molecular weight
REGNO	Organization-wide reg. no.
PUBLISH	Make available to other parts of organization--yes or no?
STORAGE_COND	Storage conditions
SOLUBILITY	Solubility
HANDLEPRECAUT	Handling precautions
STEREO_ISOMER	Whether or not there are stereo isomers
GEOM_ISOMER	Whether or not there are geometric isomers
SAM_COMMENT	Comment
LEGACY_DATE	
PARENT_REGNUM	Registration number of synthesis predecessor

TABLE 1

FIELD	INFORMATION
NUMSPECIFIC_STRUCT	Status of background calculations

Each molecule has a unique registration number, "REGNO." The remaining fields are self-explanatory. "NUMSPECIFIC_STRUCT" indicates the status of background calculations that will be described below. The information in the remaining fields is self-explanatory in the table. The present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

Another database indexed by MOLREGNO may include the two-dimensional structure for each molecule. There are many possibilities for denoting the two-dimensional structure. In one embodiment, a list of atoms and bonds is given to identify the two-dimensional structure.

A batch database may list the chemical compound containers that are available, e.g. within an organization without resort to an external ordering process. Each container within the organization may have a record within the batch database. Table 2 shows representative fields of a record within the batch database. "LOTNUM" and "REGNO" serve as a key to the batch database. It is contemplated that each container be marked with a bar code that has an associated bar code number. Certain fields concern the source of the batch. Other fields identify personnel responsible for the batch. There are also fields to represent whether certain analysis procedures have been conducted and to represent the results. Again, the present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

TABLE 2

FIELD	INFORMATION
REGNO	Reg. number for molecule
LOTNUM	Unique reg. number for batch

TABLE 2

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FIELD	INFORMATION
CHEMIST	Responsible chemist
SUPERVISOR	Responsible supervision
CHEM_SOURCE	Identify source
CATALOG NOTEBOOK	Catalog ID or NOTEBOOK#
VENDOR_NAME	Name of vendor
BARCODE	Barcode number
AMOUNT	Amount
AMOUNT_UNIT	Amount units
PURITY_PERCENT	Purity percentage
QC_METHOD	Quality control analysis method used
QC_HPLC	Chromatography applied?
HPLC_FILENAME	Chromatography results file
QC_MS	Mass spectrometry applied?
MS_FILENAME	Mass spectrometry results file
QC_C13NMR	C ₁₃ NMR applied?
C13NMR_FILENAME	C ₁₃ NMR results file
QC_HNMR	H NMR applied?
HNMR_FILENAME	H NMR results file
MPLOW	Low melting point
MPHIGH	High melting point
MP_COMMENT	Comment on melting point
BPLOW	Low boiling point
BPHIGH	High boiling point
BP_COMMENT	Boiling point comment
OPTROT	Optical rotation information

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TABLE 2

FIELD	INFORMATION
PHYS STATE	Liquid, solid, or gas
BATCH COMMENT	Batch comment
HANDLE PRECAUT	Handling precautions
STOR COND	Storage conditions
ASSIGNED_OTHER_ REGNO	Other Organization reg. no.
GCMS FILENAME	Gas chromatograph results
QC_GCMS	Gas chromatography applied?
LOCATION	Room
PLACEMENT	Position within room

The databases are preferably maintained as Oracle relational databases at central station 202. External access to the databases is provided by the Enterprise Server program available from Netscape.

Registry System

Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to the present invention. This registration system allows users to register proprietary and commercially available chemical compounds into the chemical compound database. Fig. 3A depicts a top portion 300 of a registration form. Fig. 3B depicts a bottom portion 302 of this registration form. This registration form and the other displays of the interface are preferably stored at central station 202. The web browser at one of remote stations 204 requests the registration form using an HTTP request message. The HTTP request is directed to an address of central station 202 and includes an address (any identification information) of the registration form at central station 202. In response to the HTTP request, central station 202 forwards the registration form to remote station 204 for display. Central Station 202 may dynamically generate the registration form. The registration form is communicated to remote station

204 as an HTML document. This process for presenting a web-based interface may be used for all the user interfaces discussed herein.

The registration form shows locations to enter the fields of Table 2. By selecting a structure area 304, the user invokes a chemical structure drawing tool to 5 designate a two-dimensional chemical structure. By selecting a button 306, the user may reset the contents of the form. To proceed to the next screen of the registration interface, the user selects a registration preview button 308. Once the user selects registration preview button 308, the chemical compound information system compares the entered 10 two-dimensional structure of the compound to the structures of the compounds already stored in the compound database to determine if the new compound has already been registered before.

Fig. 3C depicts an upper portion 310 of a registration preview form. Fig. 3D depicts a lower portion 312 of this registration preview form. The registration preview form includes a message 314 indicating whether or not the molecule is new to 15 the compound database. Upon user selection of a commit button 316, the entered information will be added to the batch database. If the molecule is new, a new record is also added to the compound database.

Also, after the user selects commit button 316, the chemical compound information system displays a registration report form. Fig. 3E depicts an upper portion 20 318 of this registration report form. Fig. 3F depicts a lower portion 320 of this registration report form. The registration report form confirms the information that has been registered, gives a registration number 322 corresponding to "REGNO", and a time and date 324 of registration.

Operating this registry system over the web is highly beneficial. The user 25 interface is easy to use and can be accessed from any location accessible via the network. In some embodiments, the registry system operates over the Internet permitting registration to occur anywhere in the world.

Background Autonomous Enrichment

Fig. 4 is a top level flowchart describing steps of a background process for 30 enriching the compound database according to one embodiment of the present invention. The background process may operate autonomously without invocation by any user. The

background process sequentially goes through the records of the compound database (step 402) and checks if: (i) the 2 dimensional (2D) structure has been processed (step 404), and (ii) a 3 dimensional (3D) structure, corresponding to the 2D structure, has been added (step 410). If either of these have not been performed the following processes are put 5 into operation depending on which process or processes need to be done.

Preparing the 2D structure preferably involves the application of 2 processes: StripSalt (step 406) and StipProt (step 408), described below.

StripSalt:

10 Compounds obtained from commercial suppliers often contain salts which appear in the database as part of the molecule structure; this aids the laboratory chemist but interferes with structure calculations. The program stripsalt identifies disconnected fragments based on the bond connectivity data, and outputs only the largest connected fragment, which is assumed to be the molecule of interest. The technique is given in Fig. 15 5. It assumes that the structure record contains a list of covalent bonds, each of which connects 2 atoms.

20 Fig. 5 is a flowchart describing steps of removing disconnected fragments based on bond connectivity data according to one embodiment of the present invention. At step 502, the procedure starts at the first bond. At step 504, the procedure checks whether the both atoms in the bond are without a fragment label. If yes, the procedure assigns a new fragment label to both atom at step 506. If no, the procedure goes to step 508 where it checks whether only one atom in the bond has a fragment label. If yes, the procedure assigns the fragment label of the labeled atom to the unlabeled atom at step 510. If no, the procedure goes to step 512 where it checks if the fragment labels of both 25 atoms are different. If yes, the procedure goes to step 514 where it goes through every atom in the molecule and for those atoms labeled with the same fragment as the second atom in the current bond, it changes the fragment label to match the first atom in the current bond.

30 Upon a finding of no difference at step 512, and after any one of steps 506, 510, and 514, the procedure checks at step 516 whether the current bond is the last bond. If the current bond is not the last bond, the procedure goes to the next bond at step 518. If the current bond is the next bond, the procedure goes to step 520. At step 520, the

procedure counts the number of atoms in each fragment and outputs only the atoms and bonds in the largest fragment. The smaller fragment is the salt that is removed.

StripProt:

5 Frequently chemical reagents contain protecting groups which are cleaved during synthesis. It may be preferable to remove them from the database structure. This is important if the structure is used as an input to a database reaction scheme, ensuring that the resulting product structure resembles the actual chemical product. StripProt reads a set of protecting groups as chemical structures from an input file and does a 10 substructure search on the database structure. The input file also contains information about which atoms in the substructure are to be removed when a substructure match is found. The file is an ASCII file which contains a definition of its own format and as such can be modified by the user. The substructure search is an atom by atom mapping 15 algorithm as described in Gluck, D.J. "A Chemical Structure Storage and Search System Developed at Du Pont", J. Chem. Doc. 1965, 5, 43-51, the contents of which are herein incorporated by reference.

20 Generation and processing of the 3D structure involves 2 main steps: (i) calculation of 3D coordinates (step 414), and (ii) addition of pharmacophoric labels (step 412). The 3D structure is then added to the database. The 3D coordinates are calculated using the Corina program from Oxford Molecular. The pharmacophoric labels are 25 calculated by the program AddPharm, below.

Addpharm:

25 Identifies pharmacophoric groups which are relevant to drug design. They are defined as substructures in an input file which are chosen using heuristics about which substructures contain the pharmacophoric groups. For example a carboxylate has a negative charge, aliphatic amine has a positive charge, hydroxyl is both a hydrogen bond donor and acceptor, and so on. The file is an ASCII file which contains a definition 30 of its own format and can be modified by the user. The database structures are searched using the same substructure search algorithm as in StripProt. When there is a substructure hit, the file contains information about which atoms to label with which pharmacophoric type, and these are added as records in the database. The pharmacophoric groups include the following types: A: hydrogen bond acceptor, D:

hydrogen bond donor, H: hydrophobic, N: negatively charged, P: positively charged and R: aromatic. These represent the kinds of interactions observed when a small molecule ligand binds to a protein receptor. A pharmacophore is then a set of such points in a spatial arrangement which represents the interactions made with a particular protein receptor. Therefore the other procedure needed for a full pharmacophore search is a conformation generator; this may be a feature of the database or may be done by an external program.

Fig. 6 depicts a representative compound, sumatriptan succinate. The added pharmacophoric labels are shown. A succinate salt 704 can be seen to be a disconnected fragment and is therefore removed.

Compound Tracking and Acquisition

Fig. 7 is a simplified representation of a laboratory environment where systems and methods according to the present invention may be deployed. A laboratory facility 700 includes a plurality of rooms 702. Each room 702 is preferably equipped with at least one wall-mounted scanner 704 for scanning in chemical compounds. Although, Fig. 7 depicts a single scanner 704 in each room 702, there may be multiple scanners in each room. Any type of data entry device may substitute for the scanners 704. Shelves 706 store containers of chemical compounds. Each depicted room 702 is assumed to be used for experiments or chemical processing. A chemical stock room is not needed. Laboratory facility 700 is merely representative of environments where a compound tracking and acquisition system may be deployed. A compound tracking or acquisition system may be implemented in any physical environment according to the invention.

Fig. 8 depicts details of scanner 704. Scanner 704 includes a scanning wand 802 for reading bar codes from chemical compound containers. Scanning wand 802 is preferably an Intermec 1545 non-contact bar code scanner available from Intermec, Inc. of Everett, Washington. A fixed portion 804 of scanner 704 includes a display 806 for presenting user prompts, a keyboard 808, and an RF unit 810 including an antenna 812. Except for RF unit 810 and antenna 812, fixed portion 804 may be a 9560 transaction manager available from Intermec.

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In one scenario, when a container arrives in a facility receiving department, a preprinted barcode label is affixed to the outer packaging. A single box including many containers may have several labels. The containers are then initially registered in the database on central station 202. The containers are delivered to individual rooms 702 where the bar codes are scanned in. Whenever a container moves it is rescanned.

10

Fig. 9 is a flowchart describing steps of registering a new location for a chemical compound container according to one embodiment of the present invention. At step 902, a user waves wand 802 over a bar code on a chemical container. Once the bar code has been read, RF unit 810 transmits the new location information to central station 702 at step 906. RF unit 810 preferably operates around 800 MHz. Central station 202 is similarly equipped with RF receiver equipment (not shown). At step 908, central station 202 modifies the container location information in its database. Preferably, the DataConnect program available from Connectware, Inc. of Santa Clara, California interfaces between the scanner system and the databases described above.

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Optionally, a user may register consumption of compound even without change of location by scanning the bar code and making appropriate entries on keyboard 808. The user may also similarly register complete depletion of the bottle contents and automatically reorder fresh stock.

20

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Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention. Fig. 10 will be described with reference to Figs. 11A-11F which illustrate a user interface for acquiring a chemical compound. An advantage provided by virtue of the present invention is the ability to use an interface both for searching for a compound internally, and for acquiring the compound from an external source. The user interface is assumed to be active at one of remote stations 204, although it would of course be also possible to operate it at central station 202. In a preferred embodiment, the interface is web-based.

30

At step 1002, the user enters search criteria giving characteristics of the desired compound. Fig. 11A depicts the user interface for this step. The user may enter a chemical name or a chemical formula. Other textual or numerical criteria include the amount of chemical compound desired, the registration number, the catalog number or the location.

The user may also enter the structure in a structure area 1102 to find a compound having the same or similar structure to the entered structure. The user may also use structure area 1102 to specify a substructure that would be found within the desired compound. The user may also specify a configuration of pharmacaphoric groupings that can be presented by the compound as shown in Fig. 12. Fig. 12 depicts that an acceptor 1202, donor 1204, and aromatic 1206 are presented. To meet the bonding criterion determined by the depicted configuration, a compound must be able to present these pharmacaphoric groupings at the spacings indicated in Fig. 12. A pull-down menu 1104 is used to select among these various types of structural criteria.

At step 1004, central station 202 searches for compounds having the desired characteristics in the compound database and the batch database. At step 1006, remote station 204 displays the structures of compounds having characteristics matching the search criteria. A representative display for this step is depicted in Fig. 11B. For each compound the display shows a structure 1106, a registration number 1108 for the compound. When the compound is available internally, one or more location codes are also shown. When the compound is available externally, the number of suppliers 1110 is shown. Fig. 11C depicts an alternative view of the search results where more information is depicted including a molecule name 1112, a molecular formula 1114, and a molecular weight 1116.

At step 1008, by clicking on any displayed location code, the user can call up a display of a site map which the user may refer to find the physical location of the desired compound. Fig. 11D shows such a site map display 1118. In an alternative embodiment, the display may show a special icon at the location of the compound, or may show directions to the location of the compound from the user's location.

At step 1010, by clicking on the number of suppliers 1110, the user may call up a catalog display 1120 as shown in Fig. 11E. Catalog display 1120 lists vendors, and for each vendor, catalog entries for compounds satisfying the search criteria. For each catalog entry, the display may further include a purity percentage, an indicator of quantity per batch, and a price. The user may specify a desired quantity in one of quantity boxes 1122 and specify a particular catalog entry for order by clicking in one of "add to cart" boxes 1124. When the user is ready to add all of the desired catalog entries to a "virtual shopping cart," the user selects an add to cart button 1126.

Fig. 11F depicts a virtual shopping cart 1128 that lists desired compounds and their previously selected sources. Virtual shopping cart 1128 is displayed at step 1012. A current total price 1130 is given. The user can place an order for the selected items by selecting a place order button 1132. The user can also name the cart for future reference by selecting a name this cart button 1134, clear the cart by selecting a clear cart button 1136, or select a new cart by selecting a new cart button 1138. In one embodiment, when the user selects the cart, the orders are sent to a purchasing department. In another embodiment, when the user selects the cart, the orders are sent directly to the suppliers over the Internet. Payment information may be included with the electronic orders.

The result is a virtual inventory system that allows users to obtain desired compounds quickly and efficiently from both internal and external sources. Benefits include lower cost acquisition since compounds are only requested if they are not available internally, savings in search manpower, and better tracking of costs.

In the foregoing specification, the invention has been described with reference to specific exemplary embodiments thereof. It will, however, be evident that various modifications and changes may be made thereunto without departing from the broader spirit and scope of the invention as set forth in the appended claims and their full scope of equivalents. For example, in any depicted flowcharts, steps may be deleted, substituted, or reordered within the scope of the present invention. Any user interface depicted as being web-based may also be implemented locally, or using any network protocol. For web-based implementations, links may be provided among any combination of the user interface displays to permit free navigation.

WHAT IS CLAIMED IS:

1 1. A computer-implemented method for operating a chemical
2 compound database, said method comprising:

3 accepting input from a user specifying a two-dimensional structure of a
4 chemical compound;

5 storing said two-dimensional chemical structure in a chemical compound
6 database;

7 autonomously retrieving said two-dimensional chemical structure from
8 said chemical compound database as part of a background database management process;
9 and

10 autonomously invoking a three-dimensional structure evaluation routine
11 to determine a three-dimensional structure of said compound based on said two-
12 dimensional chemical structure as a part of said background database management
13 process.

1 2. A computer-implemented method for operating a chemical
2 compound database, said method comprising:

3 accepting input from a user specifying a two-dimensional structure of a
4 chemical compound;

5 storing said two-dimensional chemical structure in a chemical compound
6 database;

7 autonomously retrieving said two-dimensional chemical structure from
8 said chemical compound database as part of a background database management process;
9 and

10 autonomously processing said two-dimensional chemical structure to
11 remove salts from said two-dimensional chemical structure.

1 3. A computer-implemented method for operating a chemical
2 compound database, said method comprising:

3 accepting input from a user specifying a two-dimensional structure of a
4 chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said two-dimensional chemical structure to remove protective groups from said two-dimensional chemical structure.

4. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database and 3D structures;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said 3D-dimensional chemical structure to identify pharmacophores in said 3D-dimensional chemical structure.

5. A computer-implemented method for facilitating acquisition of chemical compounds comprising the steps of:

operating an available compound database identifying chemical compounds available within an organization;

accepting user input identifying a desired chemical compound;

searching for said desired chemical compound within said available compound database; and

presenting information concerning availability of said desired chemical compound within said organization and availability from at least one external source.

1 6. The system of claim 5 wherein said database comprises a plurality
2 of records, each record associated with a particular chemical compound container and
3 indicating a last known location of said chemical compound container.

1 7. A computer-implemented method for procuring a desired chemical
2 compound comprising:

3 a) accepting user input indicating a desired chemical compound;
4 b) searching for one or more container holding said desired chemical
5 compound in a first database, said first database listing available chemical compound
6 containers and their locations; and
7 c) if no container holding said desired chemical is found in said b) step,
8 searching a second database for said desired chemical compound, said second database
9 storing ordering information for a plurality of chemical compounds.

1 8. The method of claim 7 wherein said user input comprises a name
2 of said desired chemical compound.

1 9. The method of claim 7 wherein said user input comprises a
2 chemical structure of said desired chemical compound.

1 10. The method of claim 7 wherein said user input comprises a
2 chemical substructure found within said desired chemical compound.

1 11. The method of claim 7 wherein said user input comprises a
2 chemical structure similar to a chemical structure of said desired chemical compound.

1 12. The method of claim 7 further comprising:
2 if any container of said desired chemical compound is found in said first
3 database, displaying a location of said container.

1 13. The method of claim 7 further comprising:
2 if said desired chemical compound is found in said second database,
3 displaying ordering information for said desired compound.

1 14. The method of claim 13 further comprising:
2 accepting user input ordering said desired compound; and
3 relaying said user input ordering said desired compound to a chemical
4 compound source via a network.

1 15. A computer-implemented method for registering a chemical
2 compound to a remote database comprising:
3 accepting user input at a local client specifying an address of a compound
4 input form at a remote server;
5 in response to said user input, sending a request for said compound input
6 form to said remote server;
7 in response to said request, transferring data representing said compound
8 input form from said remote server to said local client;
9 based on said data, displaying said compound input form at said local
10 client, said compound input form including fields for holding compound characteristics;
11 accepting user input at said local client specifying contents of one or more
12 of said field;
13 forwarding said contents from said local client to said remote server; and
14 adding said contents to a compound database accessible by said remote
15 server.

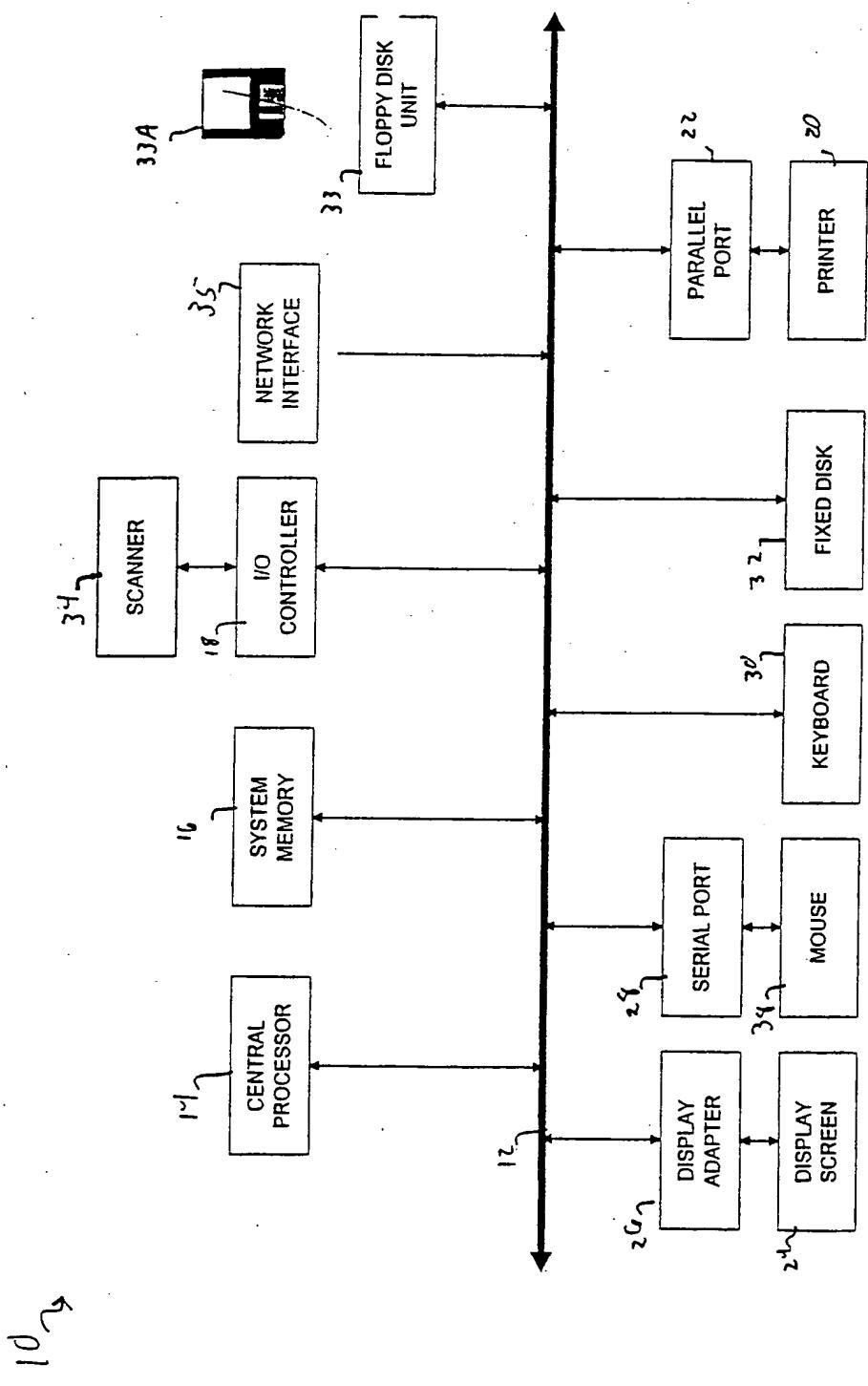


Fig. 1

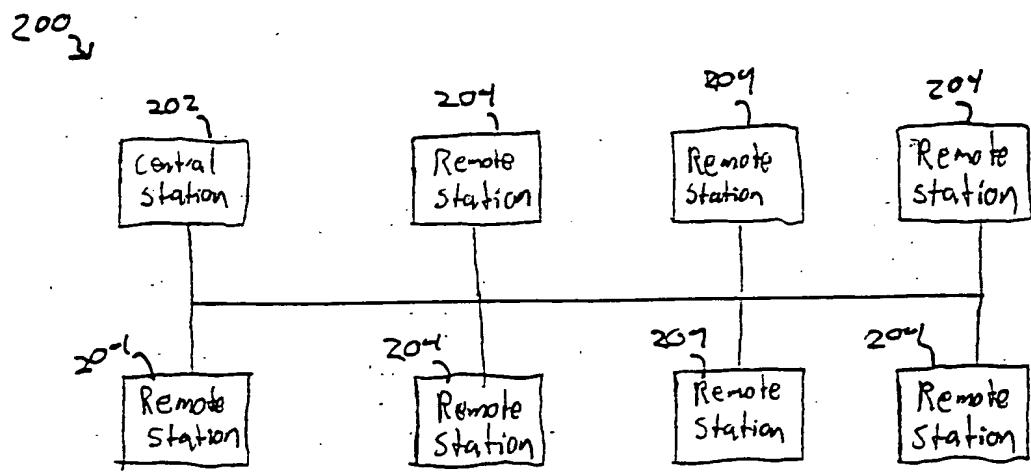
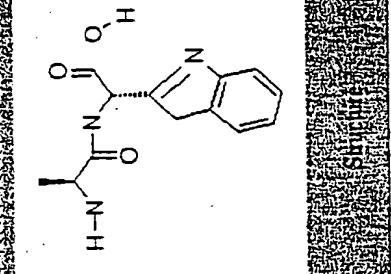


Fig. 2

Registration Form

Chemist:	<input type="text"/>	Conventional name:	<input type="text"/>
Validator:	<input type="text"/>	Stereo isomer:	<input type="text"/>
Initial Project:	<input type="text"/>	Geometrical isomer:	<input type="text"/>
Comments:	<input type="text"/>		
			

Batch Info		Batch comment	
Notebook number:	Chem_source: <input type="text"/> in house	AMOUNT: <input type="text"/> 244.0 mg	Physical state: <input type="text"/> powder
Barcode: <input type="text"/> 8765 / 66 / 77 HOOCV	Vendor name: <input type="text"/>	Optical rotation: <input type="text"/>	Comment on the melting point: <input type="text"/>
Melting point: <input type="text"/> - <input type="text"/> °C	Boiling point: <input type="text"/> - <input type="text"/> °C	Comment on the boiling point: <input type="text"/>	Comment on the melting point: <input type="text"/>
Directions: <input type="text"/>			

Fig. 3A

Purity:	99.0	%
Purity method:	HPLC	
Recommended Bioassay Solvent:		
Handling Precautions:		
Protection from heat and light <input checked="" type="checkbox"/>		
Storage Conditions:		
RT <input checked="" type="checkbox"/>		
Analytical method Yes/No File Name:		
HPLC:	<input checked="" type="checkbox"/>	109140-2
Mass Spectra:	<input checked="" type="checkbox"/>	H935064
H NMR:	<input type="checkbox"/>	
C13 NMR:	<input type="checkbox"/>	
GCMS:	<input type="checkbox"/>	
Location <input checked="" type="checkbox"/>		
Placement <input checked="" type="checkbox"/>		

302

Fig. 3D

Registration Preview Form

The molecule is new to the database.

The structure and batchinfo will be registered if you commit.



ChemBank sample info:

Molregno number is:	no info	Conventional name:	
Chemist:	Charlie Peng	Stereo isomer:	
Validator:	Steve Muskal	Geometrical isomer:	
Initial Project:		Comments:	
Molecular weight:		Structure	
not calculated yet			
Molecular formula:			
not calculated yet			

310

Fig. 3C

✓312

OI: A9765/66/77 LOTNUK, not	Barcode: HOOHCV Chem_source: In house	AMOUNT: 244.0mg	Batch comment:																		
Melting point: - °C	Boiling point: - °C	Optical rotation:	Physical state: powder																		
Comment on the melting point:	Comment on the boiling point:	Handling Precautions: Protect from heat and light																			
Purity: 99.0% Purity method: HPLC		Storage Conditions: RT																			
<table border="1"> <tr> <th>Analytical method</th> <th>Yes/No</th> <th>File Name</th> </tr> <tr> <td>HPLC:</td> <td>Y</td> <td>A09140-2</td> </tr> <tr> <td>Mass Spectra</td> <td>Y</td> <td>M935064</td> </tr> <tr> <td>H NMR:</td> <td>N</td> <td></td> </tr> <tr> <td>C13 NMR:</td> <td>N</td> <td></td> </tr> <tr> <td>GCMS:</td> <td>N</td> <td></td> </tr> </table>				Analytical method	Yes/No	File Name	HPLC:	Y	A09140-2	Mass Spectra	Y	M935064	H NMR:	N		C13 NMR:	N		GCMS:	N	
Analytical method	Yes/No	File Name																			
HPLC:	Y	A09140-2																			
Mass Spectra	Y	M935064																			
H NMR:	N																				
C13 NMR:	N																				
GCMS:	N																				

Fig. 3D

ChemBank Registration Report Form

321 month date year time:

Your assigned compound registration number is: CB10093

ChemBank sample info:

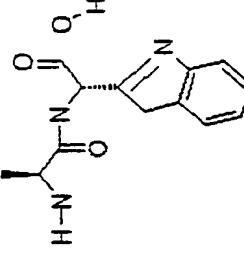
AF number is:	Conventional name:	Stereo isomer:	Geometrical isomer:	Comments:
CB10093				Structure

Fig. 3E

OI: A8763/66/77 LOTNUM:1	Barcode: HOOHCV Chem_source: in house	AMOUNT: 244mg Batch comment: null																		
Melting point 0-0 °C	Boiling point: 0-0 °C	Optical rotation: Physical state: powder																		
Comment on the melting point: Comment on the boiling point: Purity: 99% Purity method:HPLC		Handling Precautions: Protect from heat and light Storage Conditions: null																		
<table border="1"> <tr> <td>Analytical method:</td> <td>Yes/No:</td> <td>File Name:</td> </tr> <tr> <td>HPLC:</td> <td>Y</td> <td>A09140_2</td> </tr> <tr> <td>Mass Spectra:</td> <td>Y</td> <td>M935064</td> </tr> <tr> <td>1H NMR:</td> <td>N</td> <td></td> </tr> <tr> <td>C13 NMR:</td> <td>N</td> <td></td> </tr> <tr> <td>GCMS:</td> <td>N</td> <td></td> </tr> </table>			Analytical method:	Yes/No:	File Name:	HPLC:	Y	A09140_2	Mass Spectra:	Y	M935064	1H NMR:	N		C13 NMR:	N		GCMS:	N	
Analytical method:	Yes/No:	File Name:																		
HPLC:	Y	A09140_2																		
Mass Spectra:	Y	M935064																		
1H NMR:	N																			
C13 NMR:	N																			
GCMS:	N																			

320

Fig. 3F

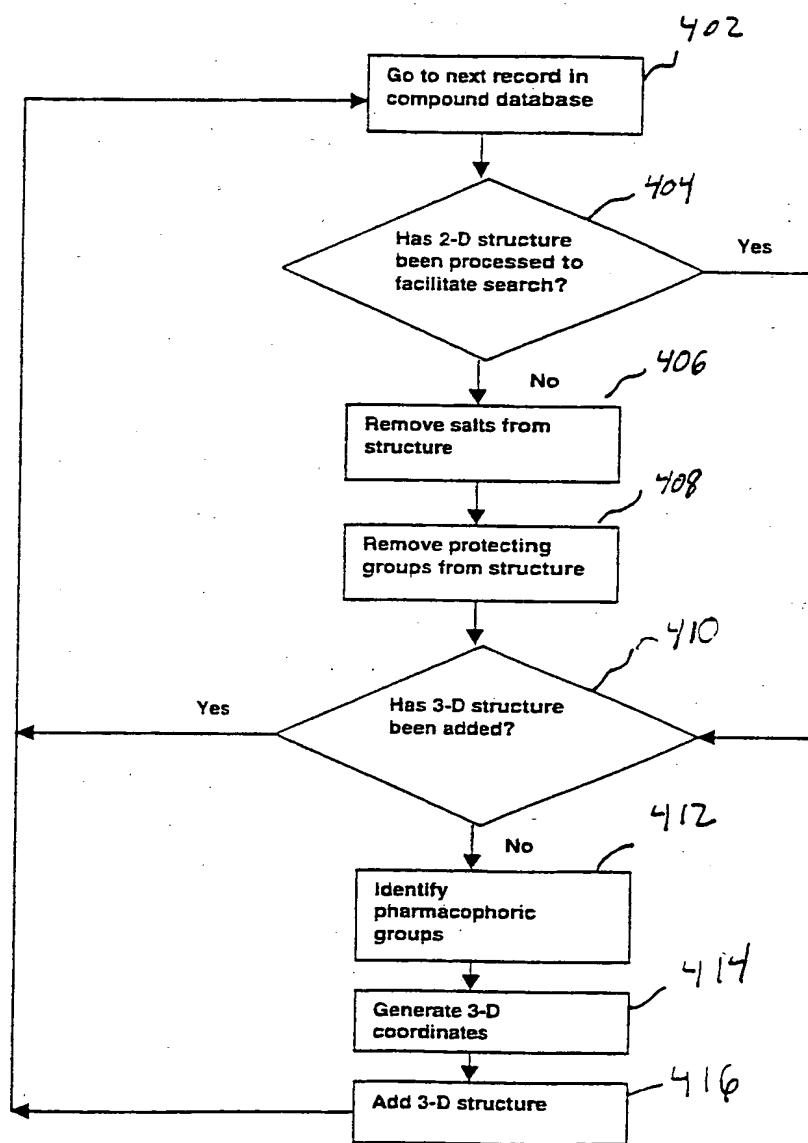


Figure 4

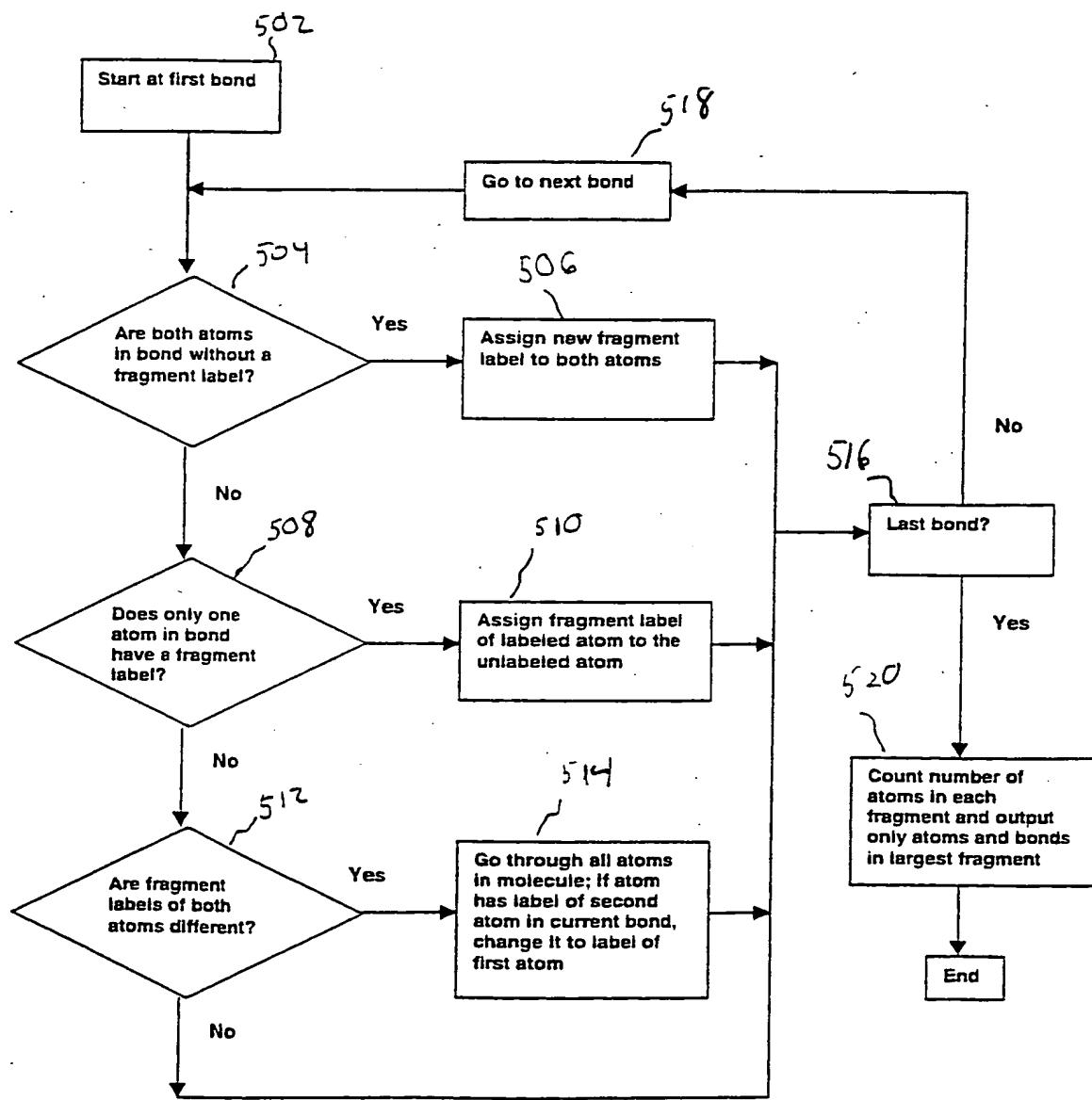
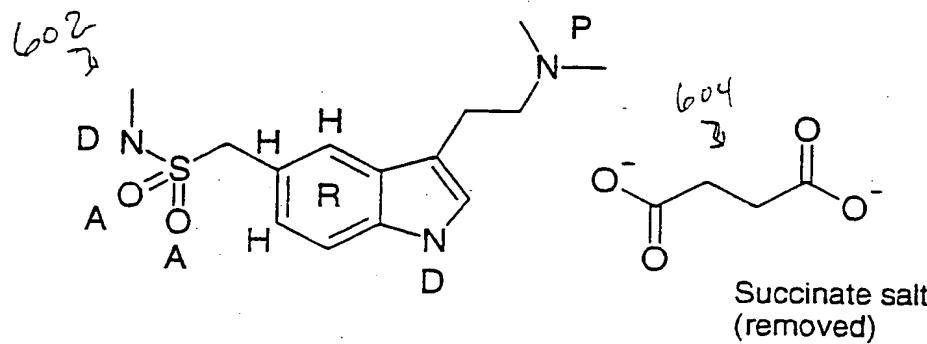


Figure 5

Sumatriptan succinate

Pharmacophore labels added:

- A : hydrogen bond acceptor
- D : hydrogen bond donor
- H : hydrophobic
- N : negative charge
- P : positive charge
- R : aromatic

Fig. 6

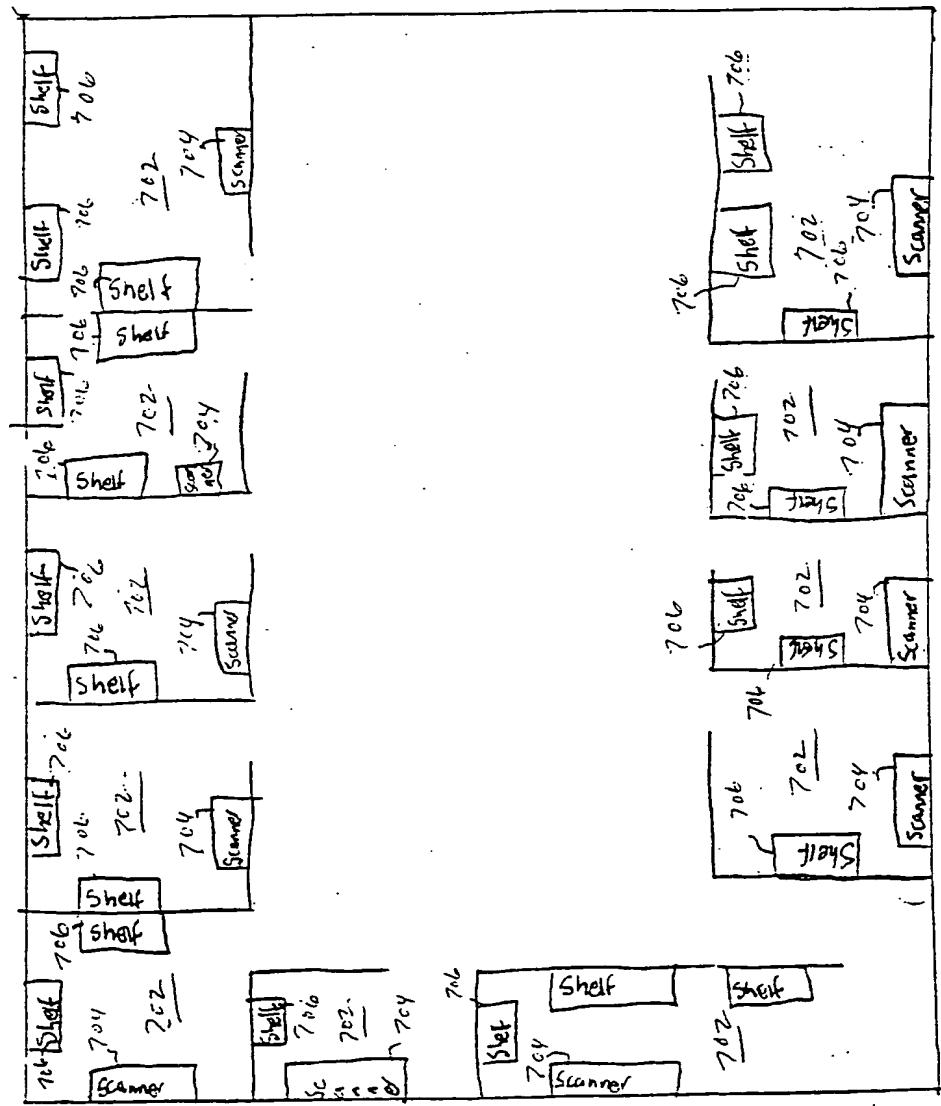


Fig. 7

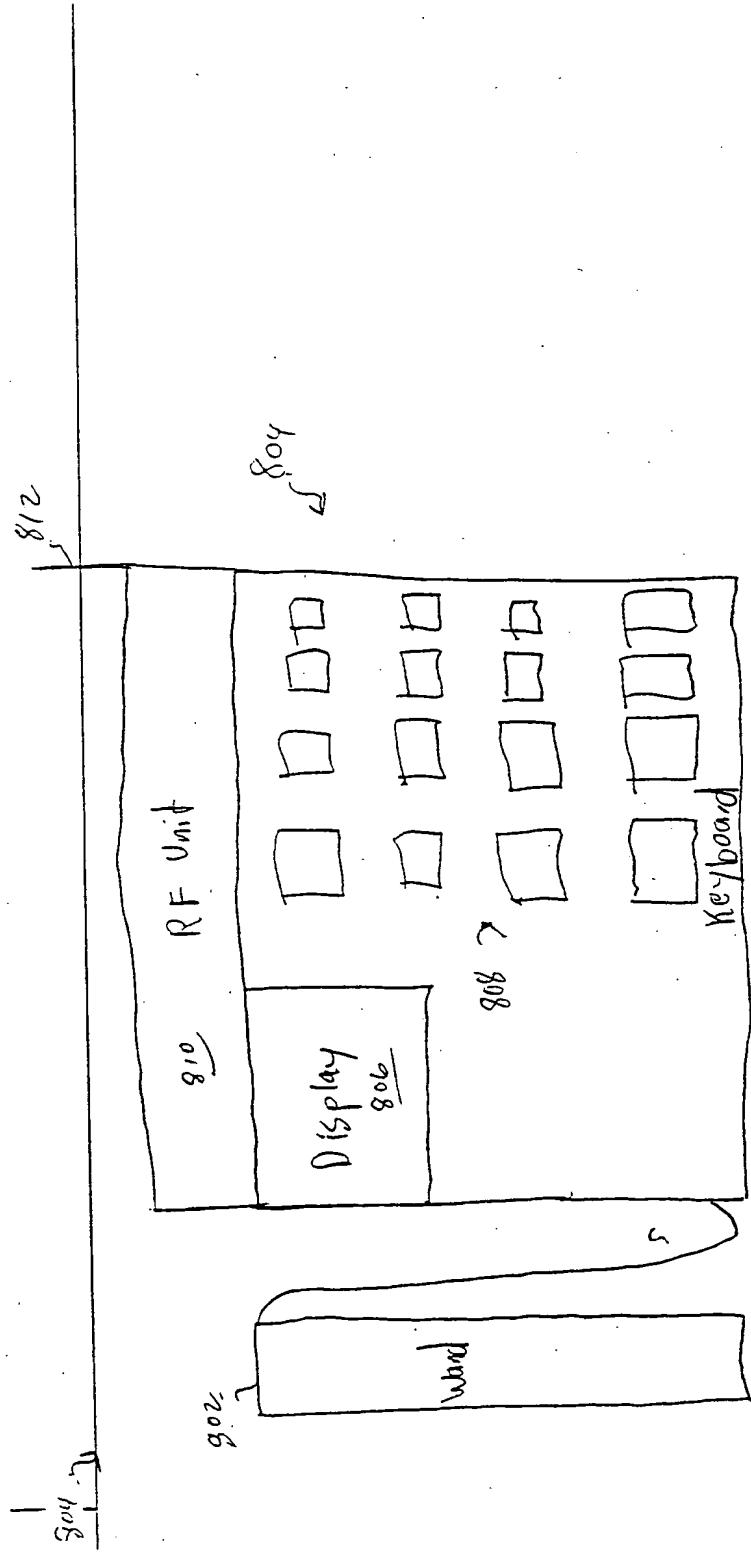
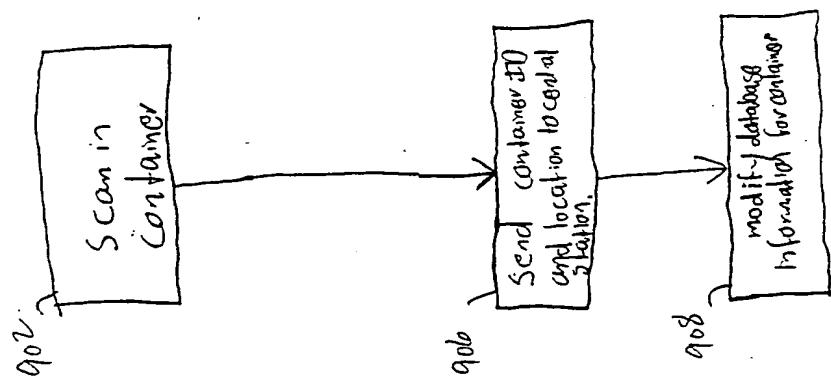


Fig. 8



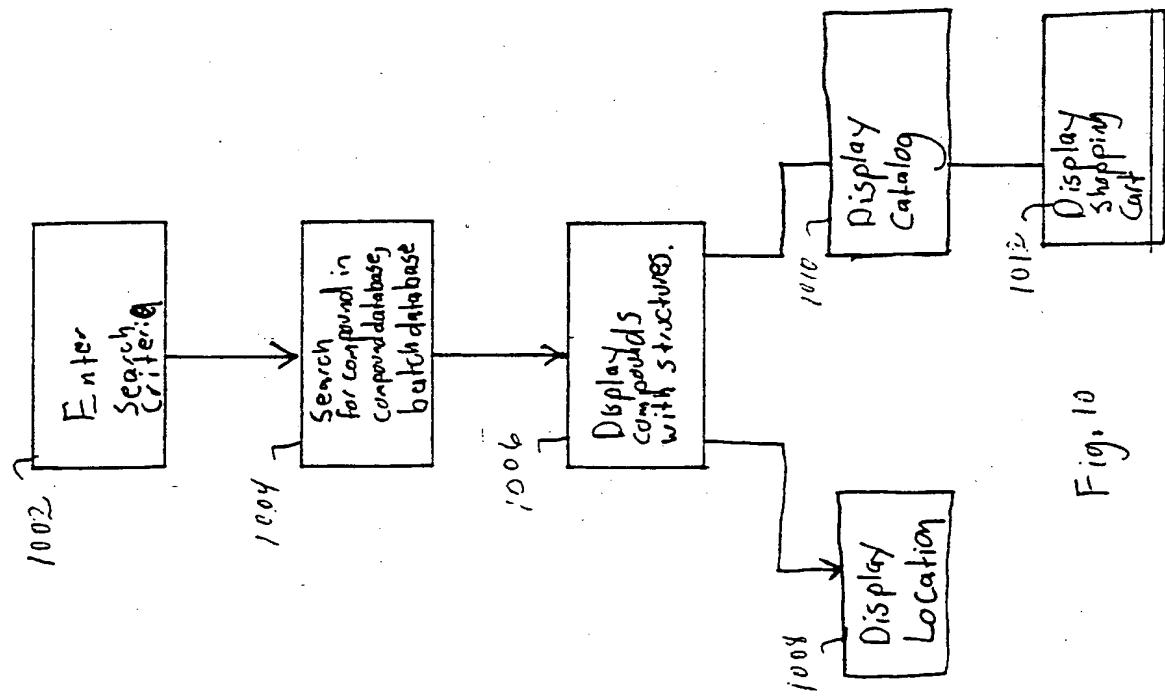
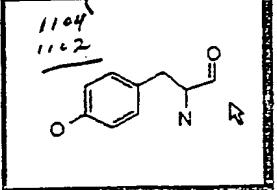


Fig. 10

Chemical Information:

Molstructure SSS

1104
1162



Name:

Formula:

Mol Weight:

Database Information:

Molecule Regno. =

Catalog Number:

Amount:

Location: Unspecified

Fig. 11A

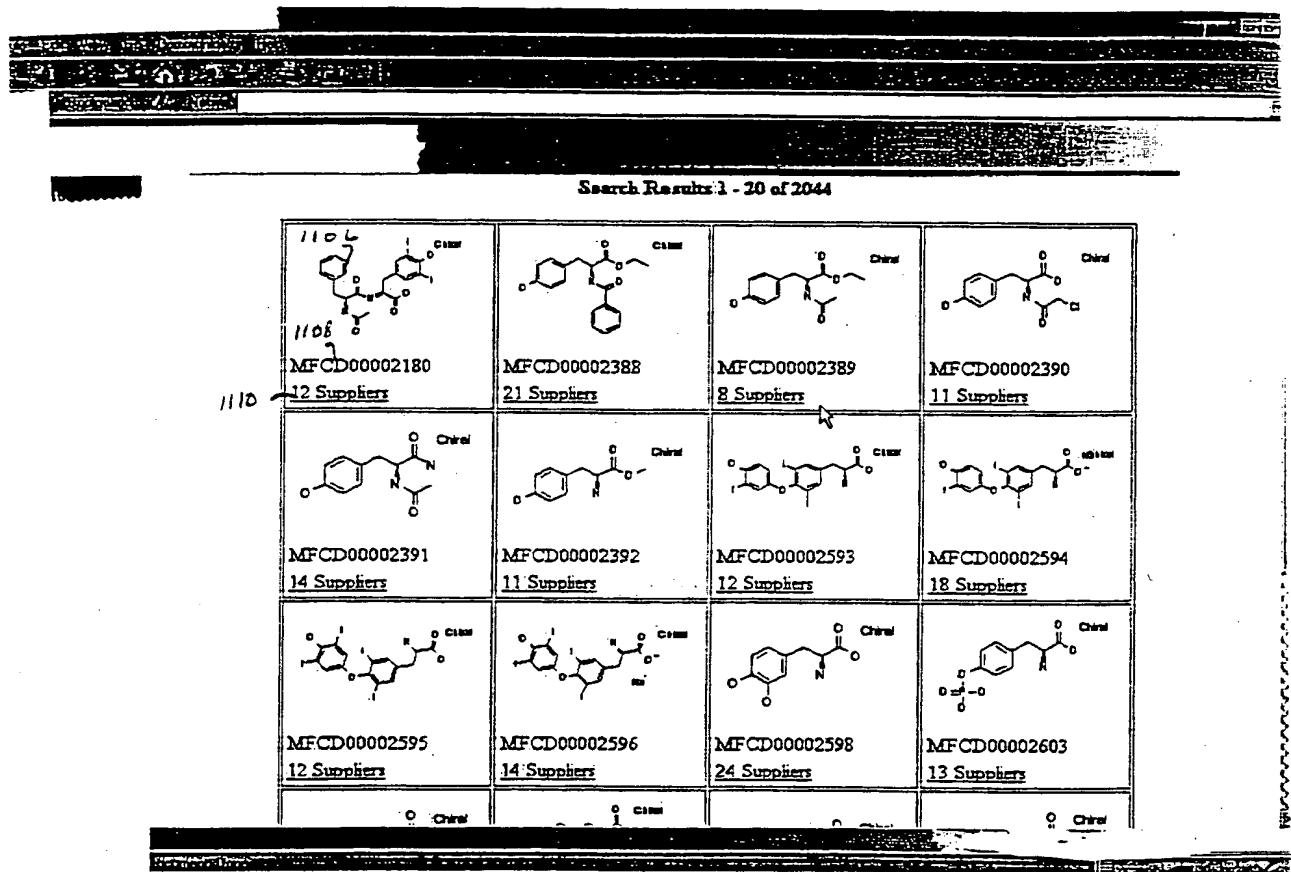


Fig. 11B

ChemStore - Netcane

Search Results 101 - 120 of 2044

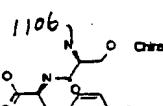
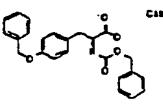
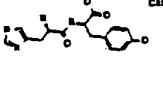
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	ACD MFCD00037819 N-CBZ-O-BENZYL-L-TYROSINE C ₁₄ H ₁₈ N ₂ O ₃ Mol Wt 405.455 7 Suppliers
	ACD MFCD00037859 HIS-TYR C ₁₂ H ₁₆ N ₂ O ₃ Mol Wt 318.335 4 Suppliers
	ACD MFCD00037870

Fig. 11c

Search Results 1 - 20 of 127057

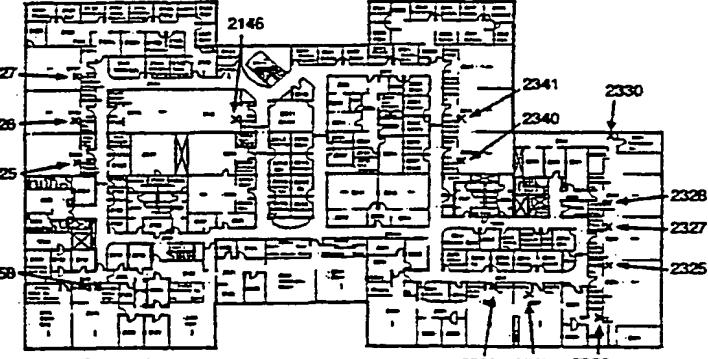
Search

- New Search
- Grid View
- Detail View

			
CB10000 E90002 SC-2001	MFCID00000001 13 Suppliers	MFCID00000004 1 Suppliers	MFCID00000005 13 Suppliers

Barcode Scanner Locations - Netscape

Location of SC-2001



3410 Santa Clara, 2nd Floor

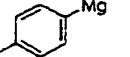
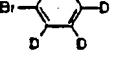

MFCID00000040 3 Suppliers

MFCID00000036 2 Suppliers

Fig. 110

1120

Availability of *N*-BENZOYL-L-TYROSINE ETHYL ESTER:

1126

Cancel

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Help

Search

New

Close

Save

Save As

Print Preview

Print

Fig. 11F

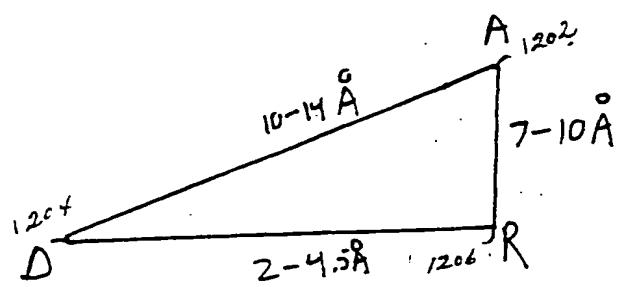


Fig. 12

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US99/15688

A. CLASSIFICATION OF SUBJECT MATTER

IPC(6) : G06F 17/30

US CL : 707/1, 100

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 707/1, 100, 3

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

APS, CAS ONLINE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	US 5,577,239 A [MOORE ET AL.] 19 NOVEMBER 1996, SEE ABSTRACT	1-15
Y	US 5,321,804 A [KUSABA ET AL.] 14 JUNE 1994, SEE ABSTRACT	1-15
A, P,	US 5,787,279 A [RIGOUTSOS] 28 JULY 1998, SEE ABSTRACT	1
A	US 5,418,944 A [DIPACE ET AL.] 23 MAY 1995, SEE ENTIRE DOCUMENT	1
A, P	US 5,812,134 A [POOSER ET AL] 22 SEPTEMBER 1998, SEE ABSTRACT.	1

Further documents are listed in the continuation of Box C.

See patent family annex.

•	Special categories of cited documents:	
•A*	document defining the general state of the art which is not considered to be of particular relevance	*T* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
•E*	earlier document published on or after the international filing date	*X* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
•L*	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	*Y* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
•O*	document referring to an oral disclosure, use, exhibition or other means	*&* document member of the same patent family
•P*	document published prior to the international filing date but later than the priority date claimed	

Date of the actual completion of the international search

27 AUGUST 1999

Date of mailing of the international search report

28 OCT 1999

Name and mailing address of the ISA/US
Commissioner of Patents and Trademarks
Box PCT
Washington, D.C. 20231

Facsimile No. (703) 305-3230

Authorized officer

SANJIV SHAH

Telephone No. (703) 305-8355

For Sanjiv Shah

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International Bureau(43) International Publication Date
20 January 2000 (20.01.2000)

PCT

(10) International Publication Number
WO 00/03336 A1

(51) International Patent Classification⁶: G06F 17/30 (72) Inventors; and
 (21) International Application Number: PCT/US99/15688 (75) Inventors/Applicants (for US only): MUSKAL, Steven, Marc [US/US]; 2656 Hesselbein Way, San Jose, CA 95148 (US). EGLI, Paul, Andrew [US/US]; 39865 Cedar Boulevard #342, Newark, CA 94560 (US). PENG, Chunyang [CN/US]; 20650 Park Circle E. #1, Cupertino, CA 95014 (US). MCGREGOR, Malcolm, James [GB/US]; 655 S. Fair Oaks Avenue #G302, Sunnyvale, CA 94086 (US).

(22) International Filing Date: 12 July 1999 (12.07.1999)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data: 09/114,694 13 July 1998 (13.07.1998) US

(63) Related by continuation (CON) or continuation-in-part (CIP) to earlier application: US 09/114,694 (CIP)
Filed on 13 July 1998 (13.07.1998)

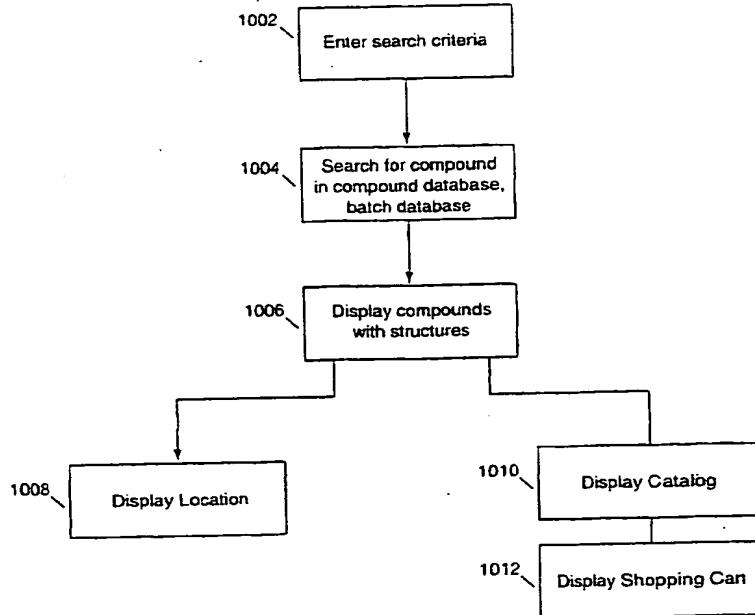
(71) Applicant (for all designated States except US): GLAXO GROUP LIMITED [GB/GB]; Glaxo Wellcome House, Berkeley Avenue, Greenford, Middlesex UB6 0NN (GB).

(74) Agent: STEVENS, Lauren, L.; Affymax Research Institute, 4001 Miranda Avenue, Palo Alto, CA 94304 (US).

(81) Designated States (national): AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW.

[Continued on next page]

(54) Title: CHEMICAL COMPOUND INFORMATION SYSTEM



WO 00/03336 A1

(57) Abstract: Systems and methods for managing chemical compound information. Chemical compound tracking and purchasing systems may be provided. A user interface (1002) allows for queries to identify compounds (1004) available internally to the organization and for orders from external sources for compounds that are unavailable internally. Background processing of compound characteristics as stored in a chemical compound database (1004) may be provided (1006).



(84) **Designated States (regional):** ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

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International Bureau(43) International Publication Date
20 January 2000 (20.01.2000)(10) International Publication Number
WO 00/003336 A1(51) International Patent Classification⁶: G06F 17/30

(21) International Application Number: PCT/US99/15688

(22) International Filing Date: 12 July 1999 (12.07.1999)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
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(CIP) to earlier application:
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Filed on 13 July 1998 (13.07.1998)(71) Applicant (for all designated States except US): GLAXO
GROUP LIMITED [GB/GB]; Glaxo Wellcome House,
Berkeley Avenue, Greenford, Middlesex UB6 0NN (GB).

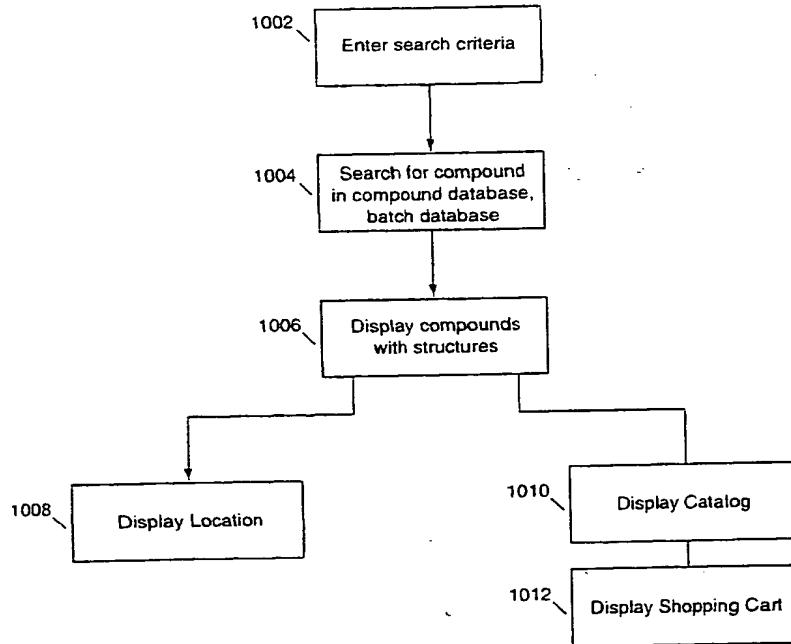
(72) Inventors; and

(75) Inventors/Applicants (for US only): MUSKAL, Steven,
Marc [US/US]; 2656 Hesselbein Way, San Jose, CA 95148
(US). EGLI, Paul, Andrew [US/US]; 39865 Cedar Boule-
vard #342, Newark, CA 94560 (US). PENG, Chunyang
[CN/US]; 20650 Park Circle E. #1, Cupertino, CA 95014
(US). MCGREGOR, Malcolm, James [GB/US]; 655 S.
Fair Oaks Avenue #G302, Sunnyvale, CA 94086 (US).(74) Agent: STEVENS, Lauren, L.; Affymax Research Insti-
tute, 4001 Miranda Avenue, Palo Alto, CA 94304 (US).(81) Designated States (national): AL, AM, AT, AU, AZ, BA,
BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES,
FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,
MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA,
ZW.

[Continued on next page]

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WO 00/003336 A1



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(84) **Designated States (regional):** ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

(15) **Information about Corrections:**

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Previous Correction:

see PCT Gazette No. 07/2001 of 15 February 2001, Section II

Published:

— *with international search report*

(48) **Date of publication of this corrected version:**

22 August 2002

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

CHEMICAL COMPOUND INFORMATION SYSTEM

5

BACKGROUND OF THE INVENTION

The present invention relates to information systems and more particularly to information systems for chemical compounds.

10 Operation of the modern chemical laboratory environment requires the management of large numbers of chemical compound containers. These containers may be dispersed over thousands of locations. A researcher or chemist desiring a given chemical compound may be aware of chemical compounds found at his or her location or possibly at nearby locations but is likely to be unaware of chemical compounds available within his or her organization. He or she may conduct a search by physically scanning available contents 15 at many locations or by making successive telephone calls to personnel throughout the organization. It may be more time efficient and thus cheaper to simply order the chemical compound from an external source even if the chemical compound is already available internally.

20 Even ordering from an external source is complicated by the need to search through numerous supplier catalogs which may not be up to date. After locating the catalog information, completing an order generally requires contacting the supplier by telephone during the supplier's business hours.

25 A related management problem concerns collecting and maintaining information on the characteristics of chemical compounds. For the purpose of identifying chemical compounds for particular purposes including pharmaceutical purposes, it would be desirable to maintain a chemical compound database that stores for each of many chemical compounds information including: 1) the three dimensional structure of the compound, 2) identification of pharmacophores of the compound, and 3) a specification of the compound structure that does not include disconnected salt fragments.

30

SUMMARY OF THE INVENTION

35 By virtue of the present invention, systems and methods for managing chemical compound information are provided. One embodiment provides a chemical compound tracking and purchasing system. A container database is maintained identifying chemical compound containers available within an organization. A integrated user interface

allows for queries to identify compounds available internally to the organization and for orders from external sources for compounds that are unavailable internally.

Another embodiment of the invention provides background processing of compound characteristics as stored in a chemical compound database. When a chemical compound is registered to a database, its two-dimensional chemical structure is also registered. One or more autonomous processes take this two-dimensional chemical structure as an input to generate additional compound characteristic information to add to the compound database. For example, a first autonomous process may remove salts from stored two-dimensional structures. The removal of salts facilitates searching for useful compounds because salt substructures do not normally affect the ability of one compound to bond with another. A second autonomous process may remove protective groups from the stored structures. These are groups that cleave during synthesis and it is useful to remove them from the compound database to facilitate the evaluation of database products. A third autonomous process may determine a possible three-dimensional structure for each compound, an example of information useful in identifying compounds having desired pharmaceutical characteristics. A fourth autonomous process may identify pharmacaphoric groupings in the stored two-dimensional structures. Knowledge of the pharmacaphores found within each compound greatly facilitates searching for compounds having desired pharmaceutical characteristics.

Another embodiment of the present invention provides for chemical compound registration system having a web-based interface. The web-based interface facilitates entering information about chemical compounds from any location on a network.

A further understanding of the nature and advantages of the inventions herein may be realized by reference to the remaining portions of the specification and the attached drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 depicts a computer system suitable for implementing one embodiment of the present invention.

Fig. 2 depicts a computer network suitable for implementing one embodiment of the present invention.

Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to one embodiment of the present invention.

Fig. 4 is a flowchart describing steps of an overall background process for enriching a chemical compound database in the background according to one embodiment of the present invention.

Fig. 5 is a flowchart describing steps of removing salts from a chemical compound according to one embodiment of the present invention.

Fig. 6 depicts a compound with pharmacaphoric groupings marked and with a salt removed.

Fig. 7 depicts a simplified representation of a laboratory facility.

Fig. 8 depicts a scanner as would be used in one embodiment of the present invention.

Fig. 9 depicts a flowchart describing steps of tracking chemical compound containers according to one embodiment of the present invention.

Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention.

Figs. 11A-11F depict a user interface for locating and purchasing chemical compounds according to one embodiment of the present invention.

Fig. 12 depicts a configuration of pharmacaphoric groupings.

20

DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides a chemical compound information system. In certain embodiments, the information system includes a chemical compound tracking and purchase system. In certain other embodiments, the chemical compound information system includes a chemical compound registry for registering information about new compounds. This registry may have a web-based interface. Once compounds are registered to a database, background processing may enrich the database with useful information about the compounds such as, e.g., three-dimensional structure, pharmacaphoric groupings, and information about included salts.

30

Representative Hardware

Fig. 1 shows basic subsystems of a computer system suitable for use with the present invention. In Fig. 1, computer system 10 includes bus 12 which interconnects major subsystems such as central processor 14, system memory 16, input/output (I/O) controller 18, an external device such as a printer 20 via parallel port 22, display screen 24 via display adapter 26, serial port 28, keyboard 30, fixed disk drive 32 and floppy disk drive 33 operative to receive a floppy disk 33A. Many other devices can be connected such as scanning device 34 connected via I/O controller 18, a network interface 35, a mouse 38 connected via serial port 28. Many other devices or subsystems (not shown) may be connected in a similar manner. Also, it is not necessary for all of the devices shown in Fig. 1 to be present to practice the present invention, as discussed below. The devices and subsystems may be interconnected in different ways from that shown in Fig. 1. The operation of a computer system such as that shown in Fig. 1 is readily known in the art and is not discussed in detail in the present application. Source code to implement the present invention may be operably disposed in system memory 16 or stored on storage media such as fixed disk 32 or floppy disk 33A.

Fig. 2 depicts a computer network 200 suitable for implementing the present invention. A central station 202 maintains databases as described herein. Central station 202 is preferably a Unix or Windows NT server such as an ORGIN 2000 server available from Silicon Graphics, Inc. of Mountain View, California. Central station 202 operates databases as described below and preferably provides external access to these databases using standard well-known Internet protocols such as HTTP. Database operation may also be divided among multiple central stations.

A plurality of remote stations 204 may access the databases of central station 202 using HTTP. Database access may be for searching for needed compounds or for registering new compounds. Remote stations 204 operate standard web browsing software such as Netscape Navigator or Microsoft Internet Explorer. Remote stations 204 may be implemented on a wide variety of computer platforms that support such browsing software. Any type of network may interconnect central station 202 including LANs, WANs, the Internet, an intranet, or any combination of these.

Databases Operated

A chemical compound information system according to the present invention may maintain various databases. A chemical compound database may include records corresponding to individual chemical compounds. Each record includes one or more of the representative fields shown in Table 1.

5

TABLE 1

FIELD	INFORMATION
MOLREGNO	Unique registration number for molecule
MOLNAME	Molecule name
CONV_NAME	Conventional name
IUPAC_NAME	IUPAC name
MOLFORMULA	Molecular formula
MIN_MWT	Minimum molecular weight
MAX_MWT	Maximum molecular weight
REGNO	Organization-wide reg. no.
PUBLISH	Make available to other parts of organization--yes or no?
STORAGE_COND	Storage conditions
SOLUBILITY	Solubility
HANDLEPRECAUT	Handling precautions
STEREO_ISOMER	Whether or not there are stereo isomers
GEOM_ISOMER	Whether or not there are geometric isomers
SAM_COMMENT	Comment
LEGACY_DATE	
PARENT_REGNUM	Registration number of synthesis predecessor

TABLE 1	
FIELD	INFORMATION
NUMSPECIFIC_STRUCT	Status of background calculations

Each molecule has a unique registration number, "REGNO." The remaining fields are self-explanatory. "NUMSPECIFIC_STRUCT" indicates the status of background calculations that will be described below. The information in the remaining fields is self-explanatory in the table. The present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

Another database indexed by MOLREGNO may include the two-dimensional structure for each molecule. There are many possibilities for denoting the two-dimensional structure. In one embodiment, a list of atoms and bonds is given to identify the two-dimensional structure.

A batch database may list the chemical compound containers that are available, e.g. within an organization without resort to an external ordering process. Each container within the organization may have a record within the batch database. Table 2 shows representative fields of a record within the batch database. "LOTNUM" and "REGNO" serve as a key to the batch database. It is contemplated that each container be marked with a bar code that has an associated bar code number. Certain fields concern the source of the batch. Other fields identify personnel responsible for the batch. There are also fields to represent whether certain analysis procedures have been conducted and to represent the results. Again, the present invention contemplates omission of any or all of the listed fields or the inclusion of additional fields.

TABLE 2	
FIELD	INFORMATION
REGNO	Reg. number for molecule
LOTNUM	Unique reg. number for batch

TABLE 2

	FIELD	INFORMATION
25	CHEMIST	Responsible chemist
	SUPERVISOR	Responsible supervision
	CHEM SOURCE	Identify source
	CATALOG NOTEBOOK	Catalog ID or NOTEBOOK#
5	VENDOR NAME	Name of vendor
	Barcode	Barcode number
	AMOUNT	Amount
	AMOUNT UNIT	Amount units
	PURITY PERCENT	Purity percentage
10	QC_METHOD	Quality control analysis method used
	QC_HPLC	Chromatography applied?
	HPLC_FILENAME	Chromatography results file
	QC_MS	Mass spectrometry applied?
	MS_FILENAME	Mass spectrometry results file
15	QC_C13NMR	C ₁₃ NMR applied?
	C13NMR_FILENAME	C ₁₃ NMR results file
	QC_HNMR	H NMR applied?
	HNMR_FILENAME	H NMR results file
	MPLOW	Low melting point
20	MPHIGH	High melting point
	MP_COMMENT	Comment on melting point
	BPLOW	Low boiling point
	BPHIGH	High boiling point
	BP_COMMENT	Boiling point comment
25	OPTROT	Optical rotation information

TABLE 2

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5

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FIELD	INFORMATION
PHYS STATE	Liquid, solid, or gas
BATCH COMMENT	Batch comment
HANDLE PRECAUT	Handling precautions
STOR_COND	Storage conditions
ASSIGNED_OTHER_REGNO	Other Organization reg. no.
GCMS_FILENAME	Gas chromatograph results
QC_GCMS	Gas chromatography applied?
LOCATION	Room
PLACEMENT	Position within room

15 The databases are preferably maintained as Oracle relational databases at central station 202. External access to the databases is provided by the Enterprise Server program available from Netscape.

Registry System

20 Figs. 3A-3F depict a web-based user interface for registering chemical compounds according to the present invention. This registration system allows users to register proprietary and commercially available chemical compounds into the chemical compound database. Fig. 3A depicts a top portion 300 of a registration form. Fig. 3B depicts a bottom portion 302 of this registration form. This registration form and the other displays of the interface are preferably stored at central station 202. The web browser at one of remote stations 204 requests the registration form using an HTTP request message. The HTTP request is directed to an address of central station 202 and includes an address (any identification information) of the registration form at central station 202. In response to the HTTP request, central station 202 forwards the registration form to remote station 204 for display. Central Station 202 may dynamically generate the registration form. The registration form is communicated to remote station

204 as an HTML document. This process for presenting a web-based interface may be used for all the user interfaces discussed herein.

The registration form shows locations to enter the fields of Table 2. By selecting a structure area 304, the user invokes a chemical structure drawing tool to 5 designate a two-dimensional chemical structure. By selecting a button 306, the user may reset the contents of the form. To proceed to the next screen of the registration interface, the user selects a registration preview button 308. Once the user selects registration preview button 308, the chemical compound information system compares the entered 10 two-dimensional structure of the compound to the structures of the compounds already stored in the compound database to determine if the new compound has already been registered before.

Fig. 3C depicts an upper portion 310 of a registration preview form. Fig. 3D depicts a lower portion 312 of this registration preview form. The registration preview form includes a message 314 indicating whether or not the molecule is new to the compound database. Upon user selection of a commit button 316, the entered 15 information will be added to the batch database. If the molecule is new, a new record is also added to the compound database.

Also, after the user selects commit button 316, the chemical compound information system displays a registration report form. Fig. 3E depicts an upper portion 318 of this registration report form. Fig. 3F depicts a lower portion 320 of this registration report form. The registration report form confirms the information that has been registered, gives a registration number 322 corresponding to "REGNO", and a time and date 324 of registration.

Operating this registry system over the web is highly beneficial. The user 25 interface is easy to use and can be accessed from any location accessible via the network. In some embodiments, the registry system operates over the Internet permitting registration to occur anywhere in the world.

Background Autonomous Enrichment

Fig. 4 is a top level flowchart describing steps of a background process for 30 enriching the compound database according to one embodiment of the present invention. The background process may operate autonomously without invocation by any user. The

background process sequentially goes through the records of the compound database (step 402) and checks if: (i) the 2 dimensional (2D) structure has been processed (step 404), and (ii) a 3 dimensional (3D) structure, corresponding to the 2D structure, has been added (step 410). If either of these have not been performed the following processes are put 5 into operation depending on which process or processes need to be done.

Preparing the 2D structure preferably involves the application of 2 processes: StripSalt (step 406) and StipProt (step 408), described below.

StripSalt:

10 Compounds obtained from commercial suppliers often contain salts which appear in the database as part of the molecule structure; this aids the laboratory chemist but interferes with structure calculations. The program stripsalt identifies disconnected fragments based on the bond connectivity data, and outputs only the largest connected fragment, which is assumed to be the molecule of interest. The technique is given in Fig. 15 5. It assumes that the structure record contains a list of covalent bonds, each of which connects 2 atoms.

20 Fig. 5 is a flowchart describing steps of removing disconnected fragments based on bond connectivity data according to one embodiment of the present invention. At step 502, the procedure starts at the first bond. At step 504, the procedure checks whether the both atoms in the bond are without a fragment label. If yes, the procedure assigns a new fragment label to both atom at step 506. If no, the procedure goes to step 508 where it checks whether only one atom in the bond has a fragment label. If yes, the procedure assigns the fragment label of the labeled atom to the unlabeled atom at step 25 510. If no, the procedure goes to step 512 where it checks if the fragment labels of both atoms are different. If yes, the procedure goes to step 514 where it goes through every atom in the molecule and for those atoms labeled with the same fragment as the second atom in the current bond, it changes the fragment label to match the first atom in the current bond.

30 Upon a finding of no difference at step 512, and after any one of steps 506, 510, and 514, the procedure checks at step 516 whether the current bond is the last bond. If the current bond is not the last bond, the procedure goes to the next bond at step 518. If the current bond is the next bond, the procedure goes to step 520. At step 520, the

procedure counts the number of atoms in each fragment and outputs only the atoms and bonds in the largest fragment. The smaller fragment is the salt that is removed.

StripProt:

5 Frequently chemical reagents contain protecting groups which are cleaved during synthesis. It may be preferable to remove them from the database structure. This is important if the structure is used as an input to a database reaction scheme, ensuring that the resulting product structure resembles the actual chemical product. StripProt reads a set of protecting groups as chemical structures from an input file and does a 10 substructure search on the database structure. The input file also contains information about which atoms in the substructure are to be removed when a substructure match is found. The file is an ASCII file which contains a definition of its own format and as such 15 can be modified by the user. The substructure search is an atom by atom mapping algorithm as described in Gluck, D.J. "A Chemical Structure Storage and Search System Developed at Du Pont", J. Chem. Doc. 1965, 5, 43-51, the contents of which are herein incorporated by reference.

20 Generation and processing of the 3D structure involves 2 main steps: (i) calculation of 3D coordinates (step 414), and (ii) addition of pharmacophoric labels (step 412). The 3D structure is then added to the database. The 3D coordinates are calculated 25 using the Corina program from Oxford Molecular. The pharmacophoric labels are calculated by the program AddPharm, below.

Addpharm:

Identifies pharmacophoric groups which are relevant to drug design. They 25 are defined as substructures in an input file which are chosen using heuristics about which substructures contain the pharmacophoric groups. For example a carboxylate has a negative charge, aliphatic amine has a positive charge, hydroxyl is both a hydrogen bond donor and acceptor, and so on. The file is an ASCII file which contains a definition 30 of its own format and can be modified by the user. The database structures are searched using the same substructure search algorithm as in StripProt. When there is a substructure hit, the file contains information about which atoms to label with which pharmacophoric type, and these are added as records in the database. The pharmacophoric groups include the following types: A: hydrogen bond acceptor, D:

hydrogen bond donor, H: hydrophobic, N: negatively charged, P: positively charged and R: aromatic. These represent the kinds of interactions observed when a small molecule ligand binds to a protein receptor. A pharmacophore is then a set of such points in a spatial arrangement which represents the interactions made with a particular protein receptor. Therefore the other procedure needed for a full pharmacophore search is a conformation generator; this may be a feature of the database or may be done by an external program.

Fig. 6 depicts a representative compound, sumatriptan succinate. The added pharmacophoric labels are shown. A succinate salt 704 can be seen to be a disconnected fragment and is therefore removed.

Compound Tracking and Acquisition

Fig. 7 is a simplified representation of a laboratory environment where systems and methods according to the present invention may be deployed. A laboratory facility 700 includes a plurality of rooms 702. Each room 702 is preferably equipped with at least one wall-mounted scanner 704 for scanning in chemical compounds. Although, Fig. 7 depicts a single scanner 704 in each room 702, there may be multiple scanners in each room. Any type of data entry device may substitute for the scanners 704. Shelves 706 store containers of chemical compounds. Each depicted room 702 is assumed to be used for experiments or chemical processing. A chemical stock room is not needed. Laboratory facility 700 is merely representative of environments where a compound tracking and acquisition system may be deployed. A compound tracking or acquisition system may be implemented in any physical environment according to the invention.

Fig. 8 depicts details of scanner 704. Scanner 704 includes a scanning wand 802 for reading bar codes from chemical compound containers. Scanning wand 802 is preferably an Intermec 1545 non-contact bar code scanner available from Intermec, Inc. of Everett, Washington. A fixed portion 804 of scanner 704 includes a display 806 for presenting user prompts, a keyboard 808, and an RF unit 810 including an antenna 812. Except for RF unit 810 and antenna 812, fixed portion 804 may be a 9560 transaction manager available from Intermec.

5 In one scenario, when a container arrives in a facility receiving department, a preprinted barcode label is affixed to the outer packaging. A single box including many containers may have several labels. The containers are then initially registered in the database on central station 202. The containers are delivered to individual rooms 702 where the bar codes are scanned in. Whenever a container moves it is rescanned.

10 Fig. 9 is a flowchart describing steps of registering a new location for a chemical compound container according to one embodiment of the present invention. At step 902, a user waves wand 802 over a bar code on a chemical container. Once the bar code has been read, RF unit 810 transmits the new location information to central station 202 at step 906. RF unit 810 preferably operates around 800 MHz. Central station 202 is similarly equipped with RF receiver equipment (not shown). At step 908, central station 202 modifies the container location information in its database. Preferably, the DataConnect program available from Connectware, Inc. of Santa Clara, California interfaces between the scanner system and the databases described above.

15

20 Optionally, a user may register consumption of compound even without change of location by scanning the bar code and making appropriate entries on keyboard 808. The user may also similarly register complete depletion of the bottle contents and automatically reorder fresh stock.

25 Fig. 10 is a flowchart describing steps of acquiring a chemical compound according to one embodiment of the present invention. Fig. 10 will be described with reference to Figs. 11A-11F which illustrate a user interface for acquiring a chemical compound. An advantage provided by virtue of the present invention is the ability to use an interface both for searching for a compound internally, and for acquiring the compound from an external source. The user interface is assumed to be active at one of remote stations 204, although it would of course be also possible to operate it at central station 202. In a preferred embodiment, the interface is web-based.

30 At step 1002, the user enters search criteria giving characteristics of the desired compound. Fig. 11A depicts the user interface for this step. The user may enter a chemical name or a chemical formula. Other textual or numerical criteria include the amount of chemical compound desired, the registration number, the catalog number or the location.

The user may also enter the structure in a structure area 1102 to find a compound having the same or similar structure to the entered structure. The user may also use structure area 1102 to specify a substructure that would be found within the desired compound. The user may also specify a configuration of pharmacaphoric groupings that can be presented by the compound as shown in Fig. 12. Fig. 12 depicts that an acceptor 1202, donor 1204, and aromatic 1206 are presented. To meet the bonding criterion determined by the depicted configuration, a compound must be able to present these pharmacaphoric groupings at the spacings indicated in Fig. 12. A pull-down menu 1104 is used to select among these various types of structural criteria.

At step 1004, central station 202 searches for compounds having the desired characteristics in the compound database and the batch database. At step 1006, remote station 204 displays the structures of compounds having characteristics matching the search criteria. A representative display for this step is depicted in Fig. 11B. For each compound the display shows a structure 1106, a registration number 1108 for the compound. When the compound is available internally, one or more location codes are also shown. When the compound is available externally, the number of suppliers 1110 is shown. Fig. 11C depicts an alternative view of the search results where more information is depicted including a molecule name 1112, a molecular formula 1114, and a molecular weight 1116.

At step 1008, by clicking on any displayed location code, the user can call up a display of a site map which the user may refer to find the physical location of the desired compound. Fig. 11D shows such a site map display 1118. In an alternative embodiment, the display may show a special icon at the location of the compound, or may show directions to the location of the compound from the user's location.

At step 1010, by clicking on the number of suppliers 1110, the user may call up a catalog display 1120 as shown in Fig. 11E. Catalog display 1120 lists vendors, and for each vendor, catalog entries for compounds satisfying the search criteria. For each catalog entry, the display may further include a purity percentage, an indicator of quantity per batch, and a price. The user may specify a desired quantity in one of quantity boxes 1122 and specify a particular catalog entry for order by clicking in one of "add to cart" boxes 1124. When the user is ready to add all of the desired catalog entries to a "virtual shopping cart," the user selects an add to cart button 1126.

Fig. 11F depicts a virtual shopping cart 1128 that lists desired compounds and their previously selected sources. Virtual shopping cart 1128 is displayed at step 1012. A current total price 1130 is given. The user can place an order for the selected items by selecting a place order button 1132. The user can also name the cart for future reference by selecting a name this cart button 1134, clear the cart by selecting a clear cart button 1136, or select a new cart by selecting a new cart button 1138. In one embodiment, when the user selects the cart, the orders are sent to a purchasing department. In another embodiment, when the user selects the cart, the orders are sent directly to the suppliers over the Internet. Payment information may be included with the electronic orders.

The result is a virtual inventory system that allows users to obtain desired compounds quickly and efficiently from both internal and external sources. Benefits include lower cost acquisition since compounds are only requested if they are not available internally, savings in search manpower, and better tracking of costs.

In the foregoing specification, the invention has been described with reference to specific exemplary embodiments thereof. It will, however, be evident that various modifications and changes may be made thereunto without departing from the broader spirit and scope of the invention as set forth in the appended claims and their full scope of equivalents. For example, in any depicted flowcharts, steps may be deleted, substituted, or reordered within the scope of the present invention. Any user interface depicted as being web-based may also be implemented locally, or using any network protocol. For web-based implementations, links may be provided among any combination of the user interface displays to permit free navigation.

WHAT IS CLAIMED IS:

1. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously invoking a three-dimensional structure evaluation routine to determine a three-dimensional structure of said compound based on said two-dimensional chemical structure as a part of said background database management process.

2. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said two-dimensional chemical structure to remove salts from said two-dimensional chemical structure.

3. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said two-dimensional chemical structure to remove protective groups from said two-dimensional chemical structure.

4. A computer-implemented method for operating a chemical compound database, said method comprising:

accepting input from a user specifying a two-dimensional structure of a chemical compound;

storing said two-dimensional chemical structure in a chemical compound database and 3D structures;

autonomously retrieving said two-dimensional chemical structure from said chemical compound database as part of a background database management process; and

autonomously processing said 3D-dimensional chemical structure to identify pharmacophores in said 3D-dimensional chemical structure.

5. A computer-implemented method for facilitating acquisition of chemical compounds comprising the steps of:

operating an available compound database identifying chemical compounds available within an organization;

accepting user input identifying a desired chemical compound;

searching for said desired chemical compound within said available compound database; and

presenting information concerning availability of said desired chemical compound within said organization and availability from at least one external source.

6. The system of claim 5 wherein said database comprises a plurality of records, each record associated with a particular chemical compound container and indicating a last known location of said chemical compound container.

7. A computer-implemented method for procuring a desired chemical compound comprising:

- a) accepting user input indicating a desired chemical compound;
- b) searching for one or more container holding said desired chemical compound in a first database, said first database listing available chemical compound containers and their locations; and
- c) if no container holding said desired chemical is found in said b) step, searching a second database for said desired chemical compound, said second database storing ordering information for a plurality of chemical compounds.

8. The method of claim 7 wherein said user input comprises a name of said desired chemical compound.

9. The method of claim 7 wherein said user input comprises a chemical structure of said desired chemical compound.

10. The method of claim 7 wherein said user input comprises a chemical substructure found within said desired chemical compound.

11. The method of claim 7 wherein said user input comprises a chemical structure similar to a chemical structure of said desired chemical compound.

12. The method of claim 7 further comprising:
if any container of said desired chemical compound is found in said first database, displaying a location of said container.

13. The method of claim 7 further comprising:
if said desired chemical compound is found in said second database,
displaying ordering information for said desired compound.

14. The method of claim 13 further comprising:
accepting user input ordering said desired compound; and
relaying said user input ordering said desired compound to a chemical
compound source via a network.

15. A computer-implemented method for registering a chemical
compound to a remote database comprising:
accepting user input at a local client specifying an address of a compound
input form at a remote server;
in response to said user input, sending a request for said compound input
form to said remote server;
in response to said request, transferring data representing said compound
input form from said remote server to said local client;
based on said data, displaying said compound input form at said local
client, said compound input form including fields for holding compound characteristics;
accepting user input at said local client specifying contents of one or more
of said field;
forwarding said contents from said local client to said remote server; and
adding said contents to a compound database accessible by said remote
server.

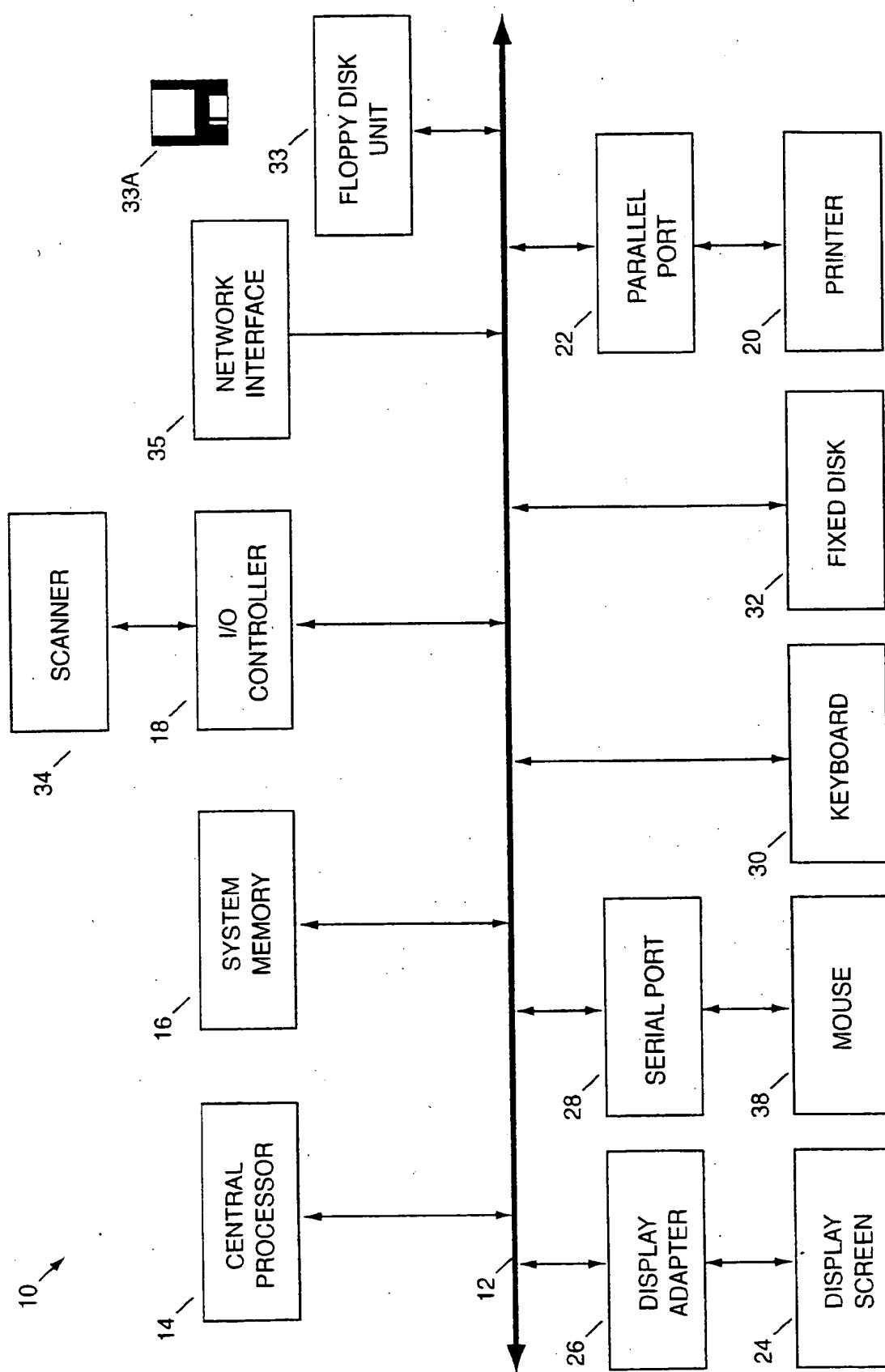


FIG. 1

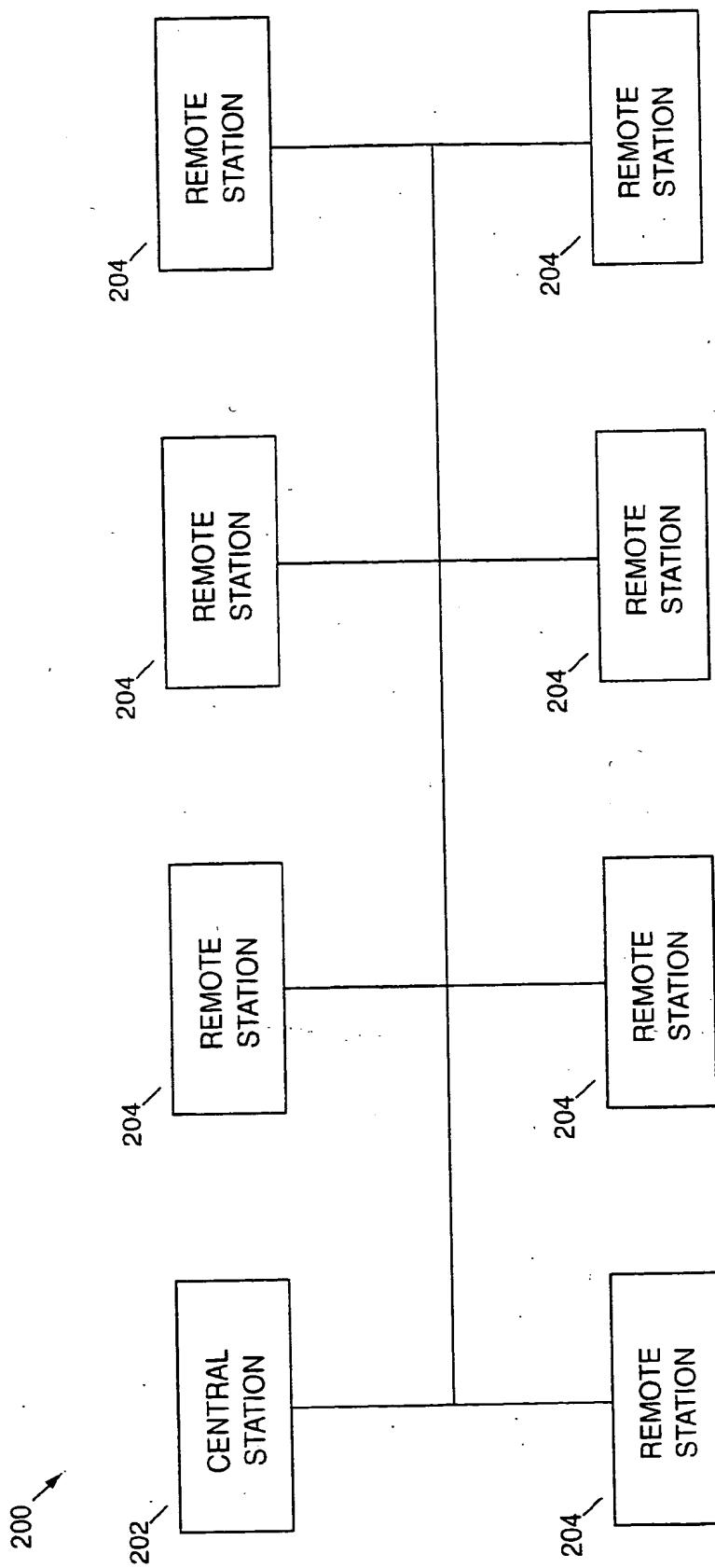


FIG. 2

Registration Form

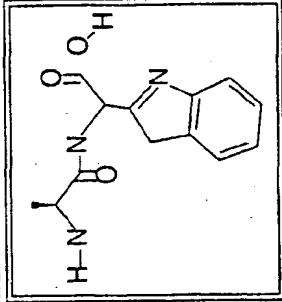
<p>Chemist: <input type="text"/></p> <p>Validator: <input type="text"/></p> <p>Initial Project: <input type="text"/></p> <p>Comments: <input type="text"/></p> <p></p> <p>Structure</p>	<p>Conventional name: <input type="text"/></p> <p>Stereo isomer: <input type="text"/></p> <p>Geometrical isomer: <input type="text"/></p>												
<p>Batch Info</p> <table border="1"> <tr> <td>Notebook number: <input type="text"/> / <input type="text"/> / <input type="text"/> / <input type="text"/> / <input type="text"/></td> <td>Chem_source: <input type="text"/> <input type="button" value="▼"/></td> <td>AMOUNT: <input type="text"/> <input type="text"/> <input type="button" value="▼"/></td> <td>Batch comment: <input type="text"/> <input type="button" value="▼"/></td> </tr> <tr> <td>Barcode: <input type="text"/></td> <td>Vendor name: <input type="text"/></td> <td>mg <input type="checkbox"/></td> <td><input type="text"/> <input type="button" value="▼"/></td> </tr> <tr> <td>Catalog number: <input type="text"/></td> <td></td> <td></td> <td></td> </tr> </table>		Notebook number: <input type="text"/> / <input type="text"/> / <input type="text"/> / <input type="text"/> / <input type="text"/>	Chem_source: <input type="text"/> <input type="button" value="▼"/>	AMOUNT: <input type="text"/> <input type="text"/> <input type="button" value="▼"/>	Batch comment: <input type="text"/> <input type="button" value="▼"/>	Barcode: <input type="text"/>	Vendor name: <input type="text"/>	mg <input type="checkbox"/>	<input type="text"/> <input type="button" value="▼"/>	Catalog number: <input type="text"/>			
Notebook number: <input type="text"/> / <input type="text"/> / <input type="text"/> / <input type="text"/> / <input type="text"/>	Chem_source: <input type="text"/> <input type="button" value="▼"/>	AMOUNT: <input type="text"/> <input type="text"/> <input type="button" value="▼"/>	Batch comment: <input type="text"/> <input type="button" value="▼"/>										
Barcode: <input type="text"/>	Vendor name: <input type="text"/>	mg <input type="checkbox"/>	<input type="text"/> <input type="button" value="▼"/>										
Catalog number: <input type="text"/>													
<p>Melting point: <input type="text"/> - <input type="text"/> °C</p> <p>Comment on the melting point: <input type="text"/> <input type="button" value="▼"/></p>	<p>Boiling point: <input type="text"/> - <input type="text"/> °C</p> <p>Comment on the boiling point: <input type="text"/> <input type="button" value="▼"/></p> <p>Optical rotation: <input type="text"/> <input type="button" value="▼"/></p>												

FIG. 3A

Purity: <input type="text" value="99.0"/>	%	Recommended Bioassay Solvent: <input type="text"/>	Handling Precautions: <input type="text" value="Protect from heat and light"/>	Storage Conditions: <input type="text" value="RT"/>																					
Purity method: <input type="text" value="HPLC"/>																									
<table border="1"><tr><td>Analytical method:</td><td>Yes/No:</td><td>File Name:</td></tr><tr><td>HPLC:</td><td><input checked="" type="checkbox"/></td><td><input type="text" value="A09140-2"/></td></tr><tr><td>Mass Spectra:</td><td><input checked="" type="checkbox"/></td><td><input type="text" value="M935064"/></td></tr><tr><td>H NMR:</td><td><input type="checkbox"/></td><td><input type="text"/></td></tr><tr><td>C13 NMR:</td><td><input type="checkbox"/></td><td><input type="text"/></td></tr><tr><td>GCMS:</td><td><input type="checkbox"/></td><td><input type="text"/></td></tr><tr><td colspan="3"><input type="button" value="Register preview"/> <input type="button" value="Reset Form"/></td></tr></table>					Analytical method:	Yes/No:	File Name:	HPLC:	<input checked="" type="checkbox"/>	<input type="text" value="A09140-2"/>	Mass Spectra:	<input checked="" type="checkbox"/>	<input type="text" value="M935064"/>	H NMR:	<input type="checkbox"/>	<input type="text"/>	C13 NMR:	<input type="checkbox"/>	<input type="text"/>	GCMS:	<input type="checkbox"/>	<input type="text"/>	<input type="button" value="Register preview"/> <input type="button" value="Reset Form"/>		
Analytical method:	Yes/No:	File Name:																							
HPLC:	<input checked="" type="checkbox"/>	<input type="text" value="A09140-2"/>																							
Mass Spectra:	<input checked="" type="checkbox"/>	<input type="text" value="M935064"/>																							
H NMR:	<input type="checkbox"/>	<input type="text"/>																							
C13 NMR:	<input type="checkbox"/>	<input type="text"/>																							
GCMS:	<input type="checkbox"/>	<input type="text"/>																							
<input type="button" value="Register preview"/> <input type="button" value="Reset Form"/>																									

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FIG. 3B

Registration Preview Form

The molecule is new to the database.

Commit

314

The structure and batchinfo will be registered if you commit.

ChemBank sample info:

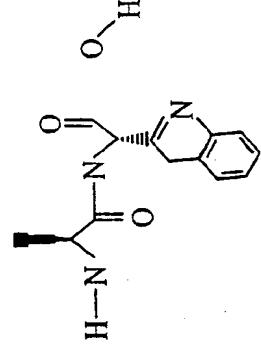
Mol regno number is:		Conventional name:
no info		Stereo isomer:
Chemist:		Geometrical isomer:
Validator:		Comments:
Initial Project:		
Molecular Weight:		
Molecular Formula:		
Structure		

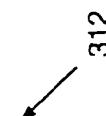
FIG. 3C

310

OI: A8765/66/77 LOTNUM: not	Barcode: HOOHCV Chem_source: in house	AMOUNT: 244.0mg	Batch comment:
Melting point: -°C	Boiling point: -°C	Optical rotation:	Physical state: powder
Comment on the melting point:	Comment on the boiling point:		
Purity: 99.0% Purity method: HPLC	Recommended Bioassay Solvent:	Handling Precautions: Protect from heat and light	Storage Conditions: RT

Analytical method:	Yes/No:	File Name:
HPLC:	Y	A09140-2
Mass Spectra	Y	M935064
H NMR:	N	
C13 NMR:	N	
GCMS:	N	

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ChemBank Registration Report Form

324 month date year time:

322
Your assigned compound registration number is: CB10093

ChemBank sample info:

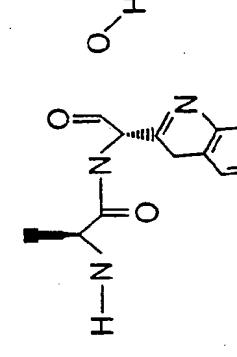
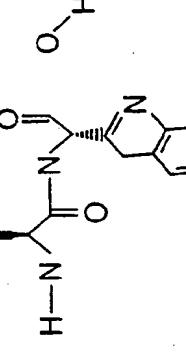
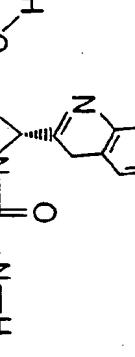
AF number is:	Conventional name:	Stereo isomer:	Geometrical isomer:	Comments:
CB10093				Structure

FIG. 3E

Or: A8765/66/77 LOTNUM: 1	Barcode: HOOHCV Chem_source: in house	AMOUNT: 244mg	Batch comment: null																		
Melting point: 0-0 °C	Boiling point: 0-0 °C	Optical rotation:	Physical state: powder																		
Comment on the melting point:	Comment on the boiling point:																				
Purity: 99% Purity method: HPLC	Recommended Bioassay Solvent: null	Handling Precautions: Protect from heat and light	Storage Conditions: RT																		
<table border="1"> <tr> <td>Analytical method:</td> <td>Yes/No:</td> <td>File Name:</td> </tr> <tr> <td>HPLC:</td> <td>Y</td> <td>A09140-2</td> </tr> <tr> <td>Mass Spectra</td> <td>Y</td> <td>M935064</td> </tr> <tr> <td>HNMR:</td> <td>N</td> <td></td> </tr> <tr> <td>C13NMR:</td> <td>N</td> <td></td> </tr> <tr> <td>GCMS:</td> <td>N</td> <td></td> </tr> </table>				Analytical method:	Yes/No:	File Name:	HPLC:	Y	A09140-2	Mass Spectra	Y	M935064	HNMR:	N		C13NMR:	N		GCMS:	N	
Analytical method:	Yes/No:	File Name:																			
HPLC:	Y	A09140-2																			
Mass Spectra	Y	M935064																			
HNMR:	N																				
C13NMR:	N																				
GCMS:	N																				

320



FIG. 3F

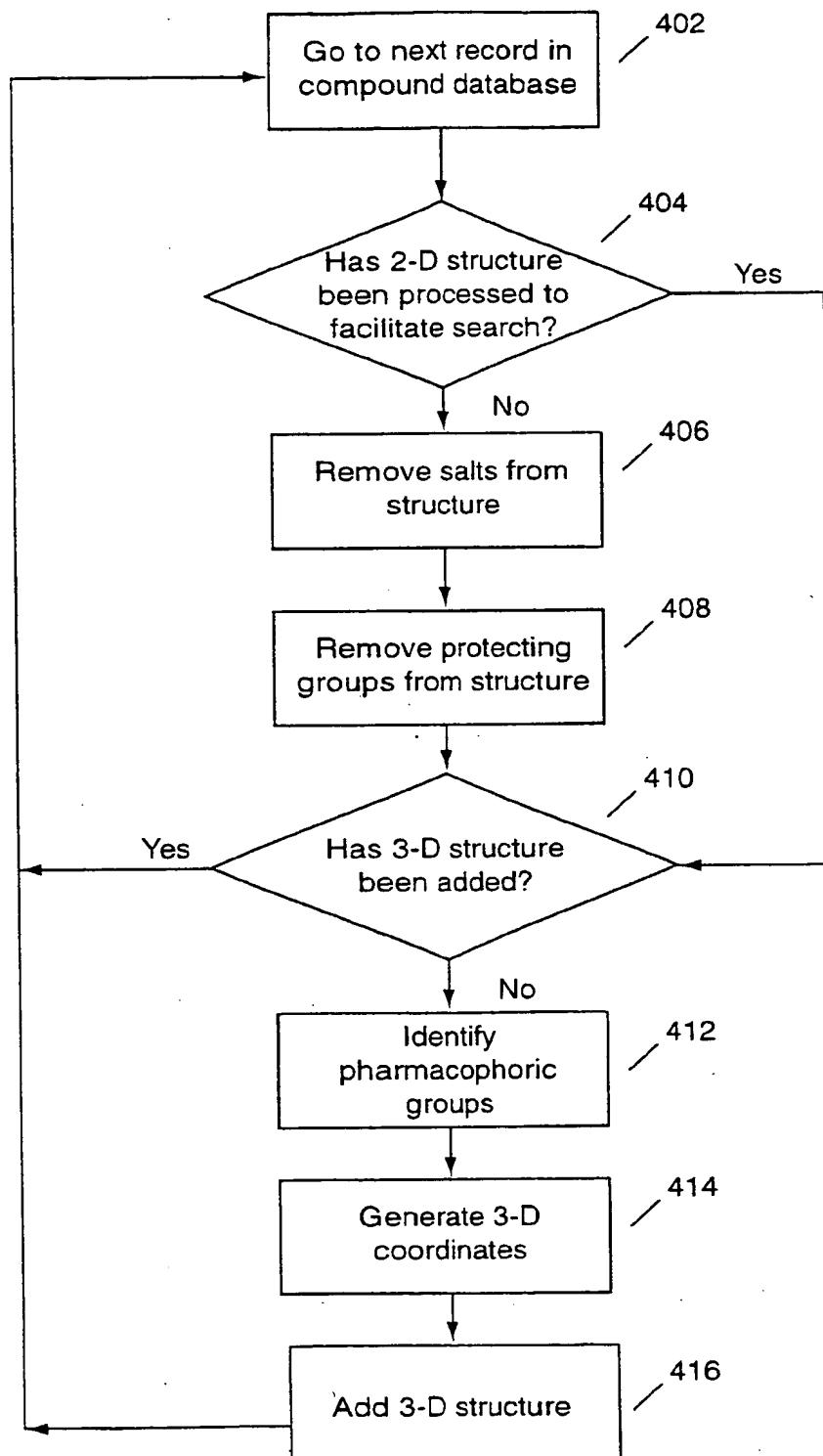


FIG. 4

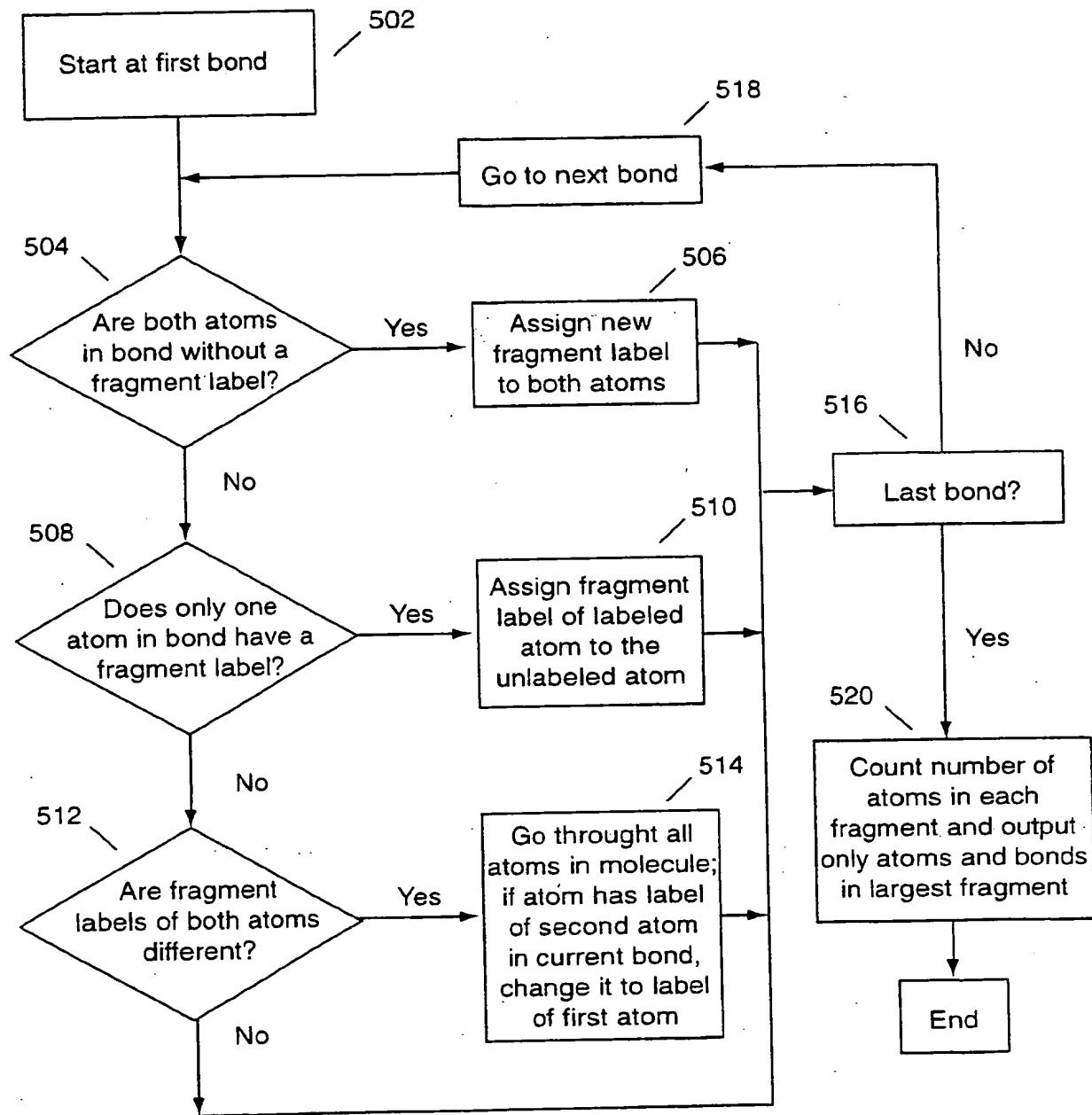
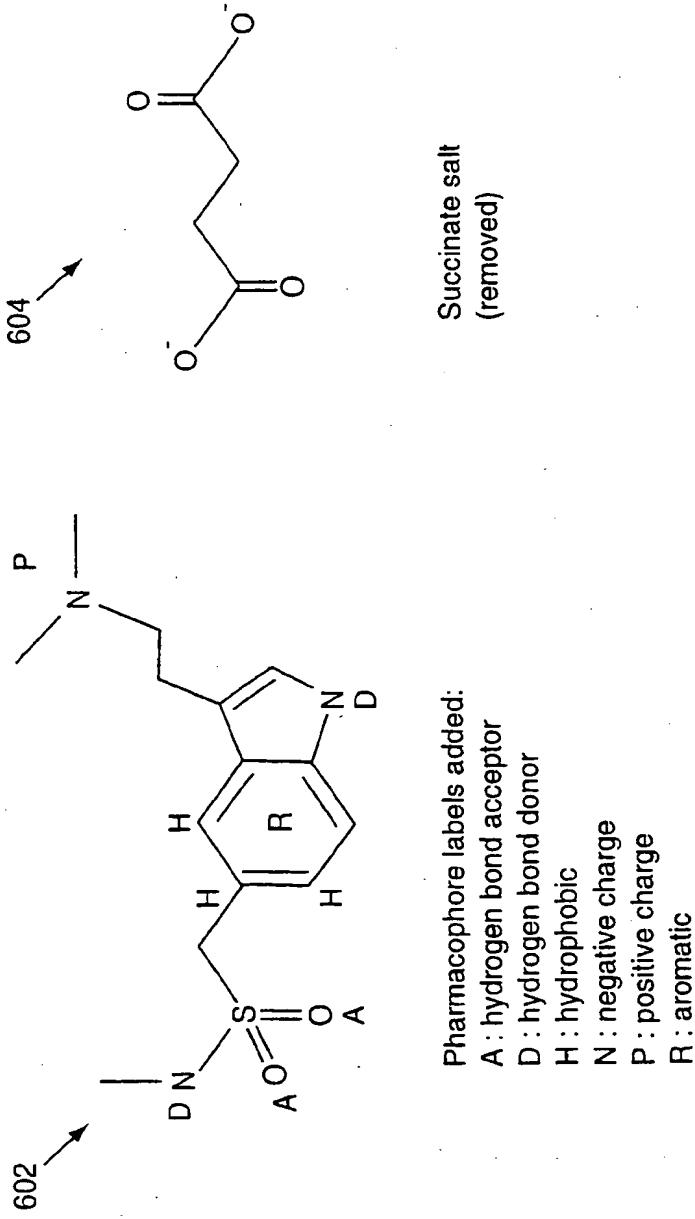


FIG. 5

Sumatriptan succinate**FIG. 6**

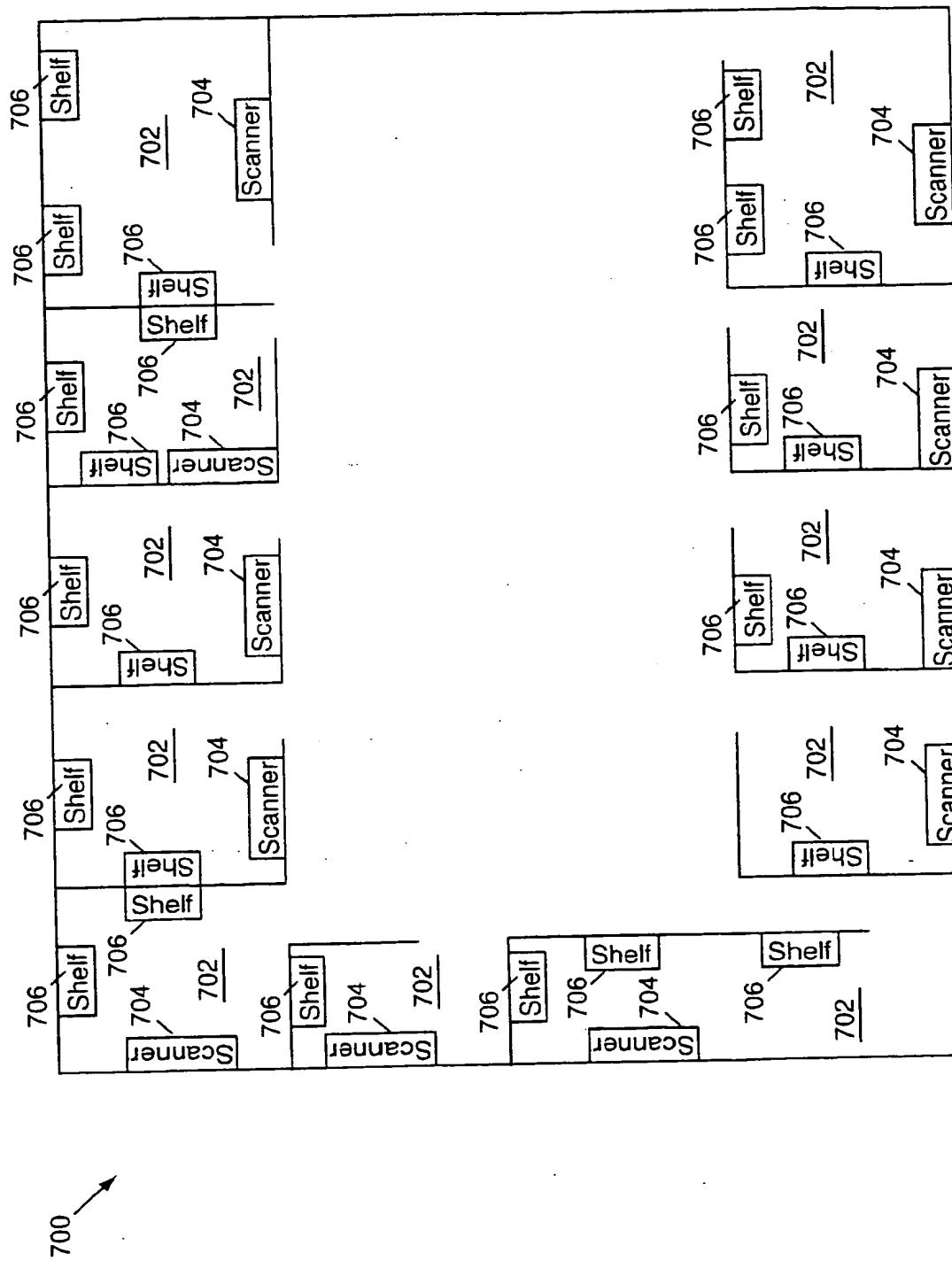


FIG. 7

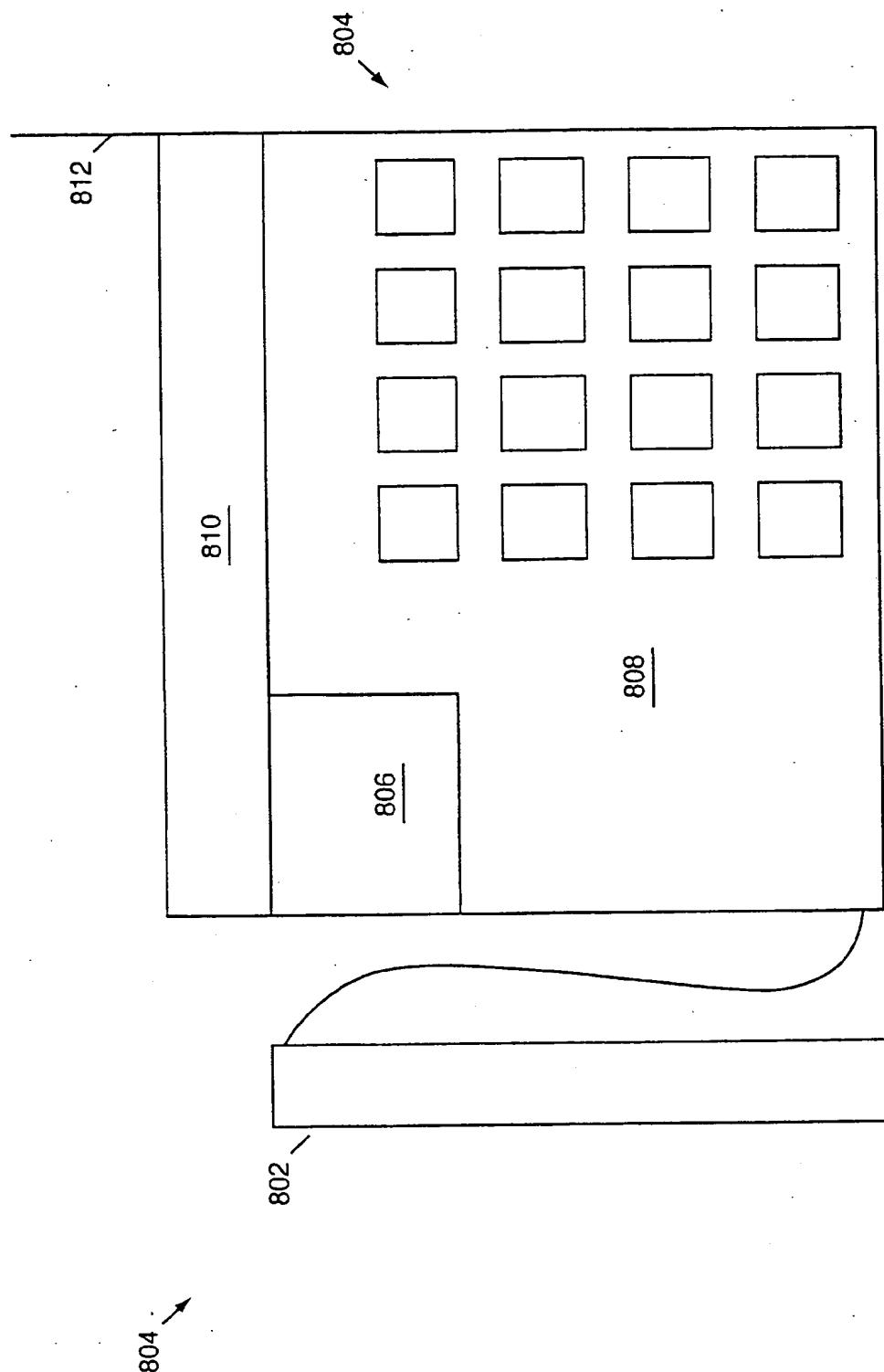


FIG. 8

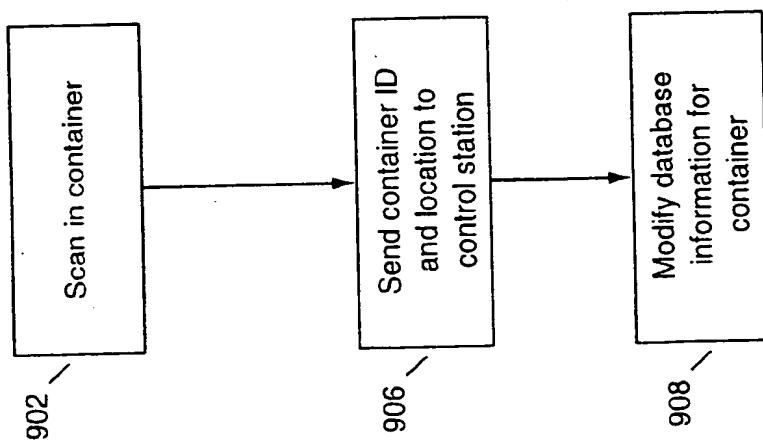


FIG. 9

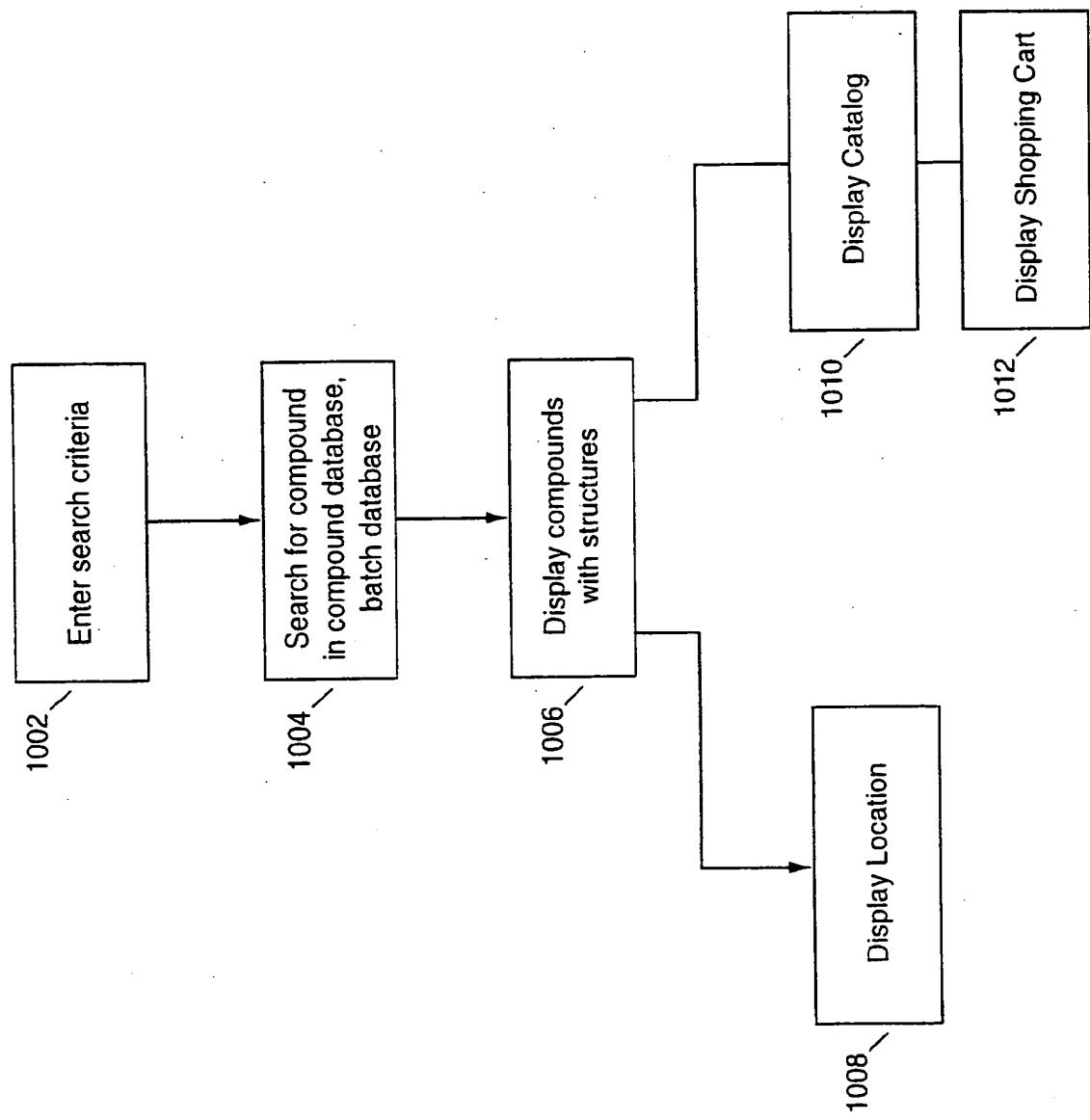
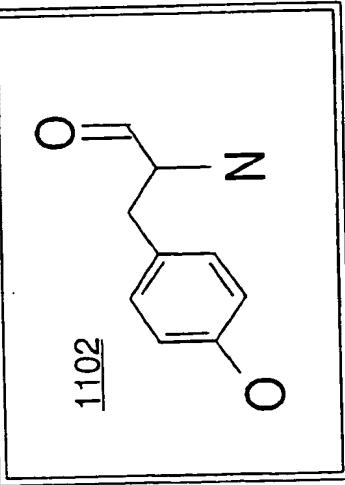


FIG. 10

1104 Chemical Information:

Name: Molstructure Name: sssName: = Formula: = Mol. Weight: =

Database Information:

Molecule Regno: = Catalog Number: = Amount: = Location: Unspecified Search Clear

FIG. 11A

Search Results 101 - 120 of 2044

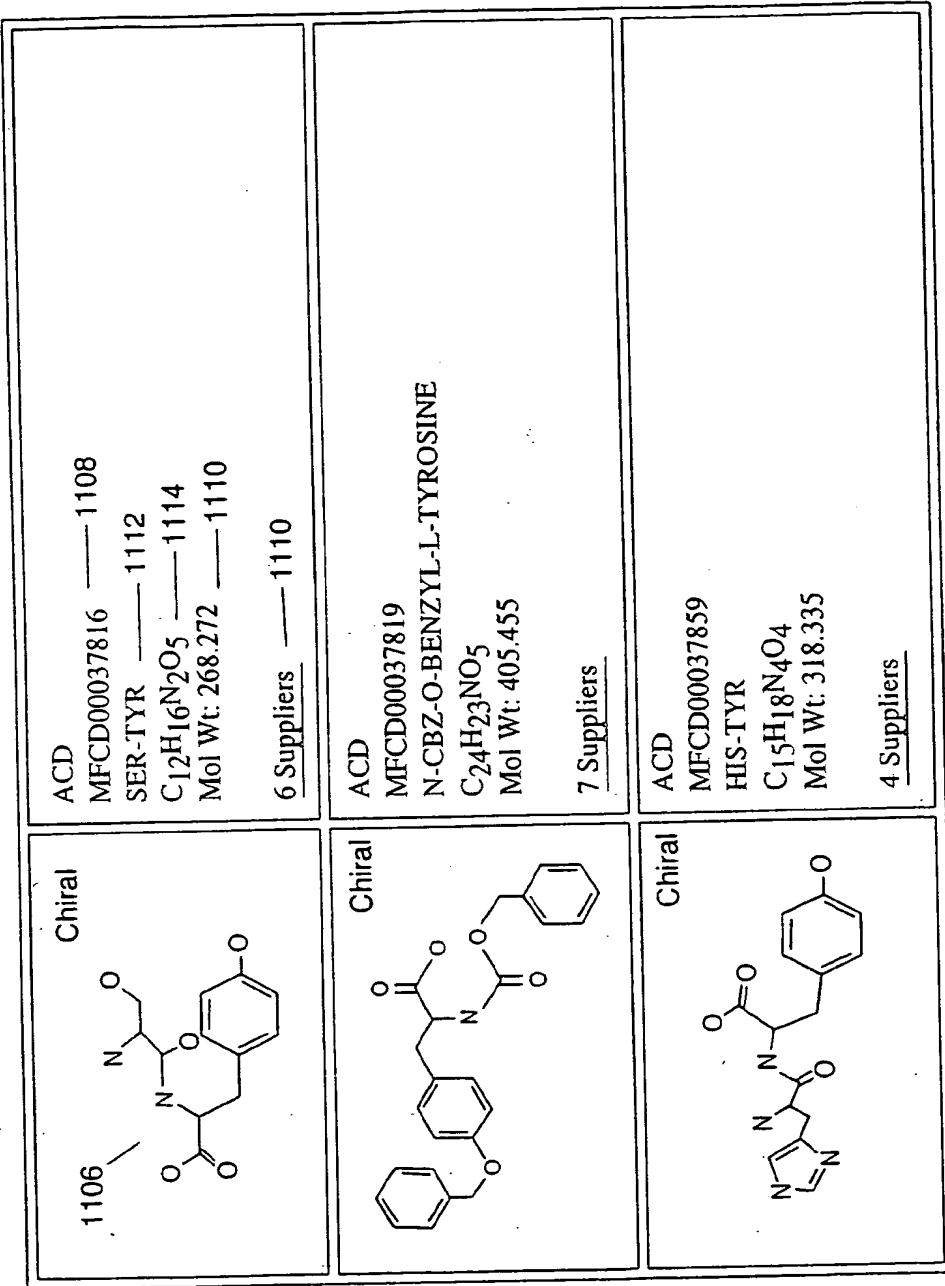


FIG. 11C

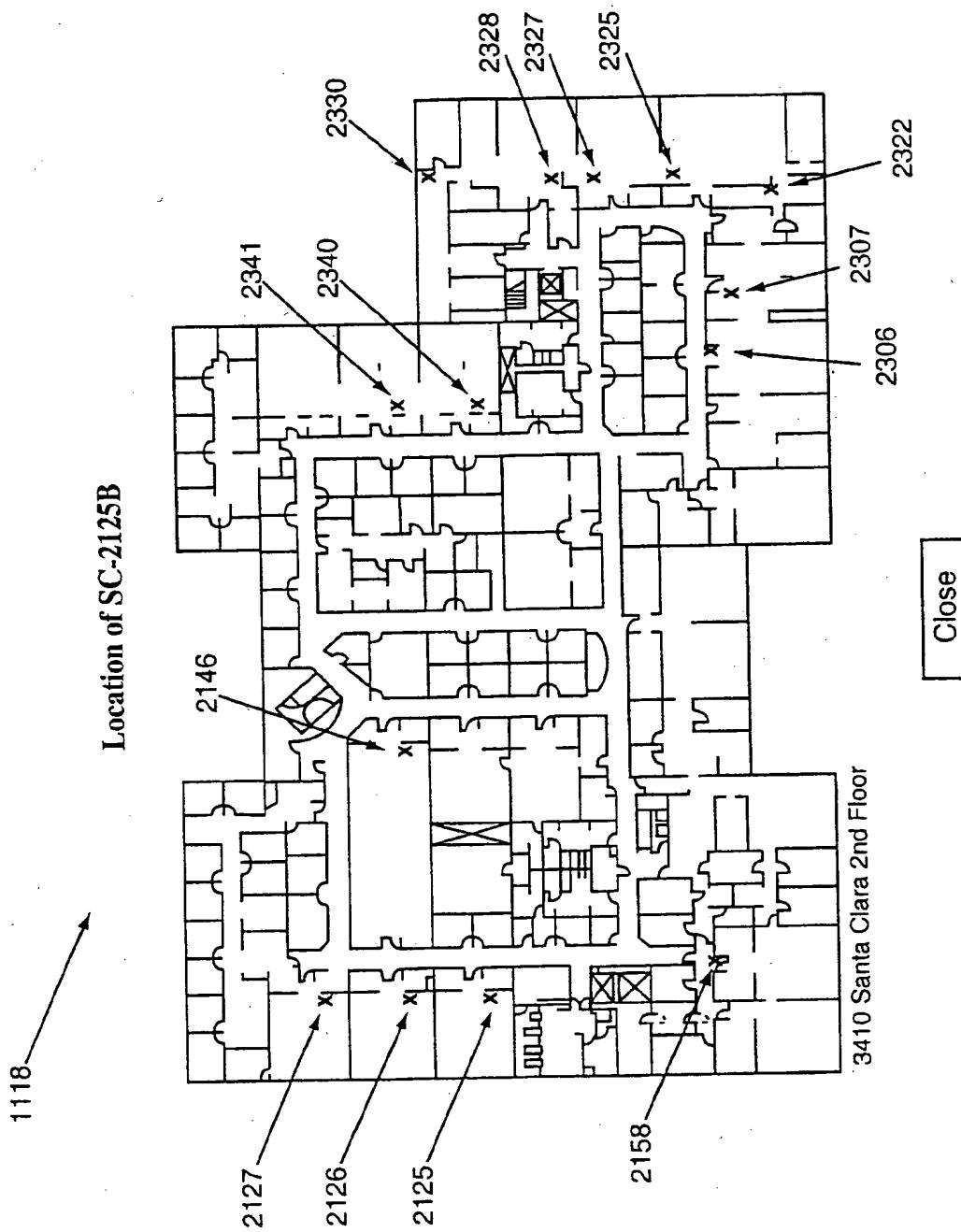


FIG. 11D

1126

Availability of N-BENZOYL-L-TYROSINE ETHYL ESTER:

Vendor	Cat #	Purity	Size	Price	Quant	Add to cart	
						1122	1124
Acros Organics	22756-0050	99%	1 GR	27.10	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Advanced ChemTech	IY7561		25 G	60.00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Aldrich Chemical Company, Inc.	IY7561		5 G	13.00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Aldrich Chemical Company, Inc.	85,658-4	98%	1 G	10.90	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Aldrich Chemical Company, Inc.	85,658-4	98%	5 G	22.10	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Apin Chemicals Ltd.	SQ19865		1	(n/a)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Bachem	SQ11928B		1	(n/a)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Bachem	E-1530		25 G	80.00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Bachem	E-1530		5 G	20.00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Bachem	E-1530		25 G	55.00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

1120

FIG. 11E

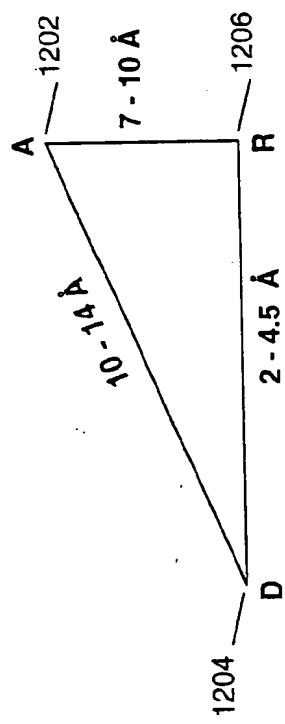


FIG. 12

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US99/15688

A. CLASSIFICATION OF SUBJECT MATTER

IPC(6) : G06P 17/30

US CL : 707/1, 100

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 707/1, 100, 3

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

APS, CAS ONLINE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	US 5,577,239 A [MOORE ET AL.] 19 NOVEMBER 1996, SEE ABSTRACT	1-15
Y	US 5,321,804 A [KUSABA ET AL.] 14 JUNE 1994, SEE ABSTRACT	1-15
A, P,	US 5,787,279 A [RIGOUTSOS] 28 JULY 1998, SEE ABSTRACT	1
A	US 5,418,944 A [DIPACE ET AL.] 23 MAY 1995, SEE ENTIRE DOCUMENT	1
A, P	US 5,812,134 A [POOSER ET AL] 22 SEPTEMBER 1998, SEE ABSTRACT.	1

 Further documents are listed in the continuation of Box C. See patent family annex.

* Special categories of cited documents:	*T*	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
A document defining the general state of the art which is not considered to be of particular relevance	*X*	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
B earlier document published on or after the international filing date	*Y*	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
L document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	*&*	document member of the same patent family
O document referring to an oral disclosure, use, exhibition or other means		
P document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search
27 AUGUST 1999Date of mailing of the international search report
28 OCT 1999Name and mailing address of the ISA/US
Commissioner of Patents and Trademarks
Box PCT
Washington, D.C. 20231
Facsimile No. (703) 305-3230Authorized officer
Fo...Bijanis Zagan
SANJIV SHAH
Telephone No. (703) 305-8355